HENRY ROYCE INSTITUTE

RESEARCH SUCCESS IN HYDROGEN

Demonstrating translational research across the hydrogen supply chain

SECOND EDITION


Vacuum
Air Pipe

FOREWORD

Hydrogen, along with its various forms of carriers, represents a genuinely transformative opportunity to decarbonise our future global energy systems using UK research solutions and industrial capabilities.

Energy-intensive industries like long-distance aerospace, marine, steel, glass, and petrochemicals, to name but a few, can't all be electrified, and present a real challenge to our net zero ambitions. Hydrogen could be used as an energy source and storage medium in these sectors, transforming our ability to tackle the climate crisis.

This is an exciting opportunity for the UK, where we have world-leading resources and capabilities which, if capitalised upon, could drive the global hydrogen industry.

The UK is now on an exciting journey to mature our capabilities and leverage our infrastructure and natural resources to capture this market. Support from government and industry has been central to drawing solutions from our diverse research community to improve the efficiency, durability, and performance monitoring of hydrogen-related technologies.

I'm proud that Royce have been at the forefront of this drive. A number of years ago, we recognised that materials solutions would be fundamental to the development of the UK and wider global hydrogen industry, and launched the "materials for end-to-end hydrogen" challenge and have since stayed an active supporter, funder and engaged party.

Led by Professor Robert Sorrell, we researched the specific challenges constraining the scaling of the hydrogen supply chain and set about funding research that will unlock the industry.

Royce has now invested £5 million in Industrial Collaboration Projects (ICPs) that match hydrogen industry players with materials researchers, producing materials solutions in commercial timescales. This second edition of our Research Success in Hydrogen publication demonstrates our continued commitment to funding truly impactful research collaborations.

The findings from the ICPs are delivering new solutions for a robust hydrogen energy system. We are delighted to share them with the wider hydrogen community and government, who are cementing hydrogen's position as a key component of our net zero journey and economic development by featuring it as part of their Clean Energy Superpower Mission.

However, developing the solutions for the hydrogen industry does not guarantee scaling – we have recognised that continued funding, endorsement, steer and clarity from government is needed alongside the commitment for early adoption at a national level. This will provide transparency on the potential for the industry and the reassurance the investment community needs.

Royce is supporting this challenge through our Royce Hydrogen Accelerator, which finds and aggregates more investment – including from overseas and private funders – for translating good ideas from this research into scalable solutions.

By continuing to collaborate on and proactively address the barriers to deployment of these essential solutions, soon the UK will be leading the way in decarbonisation using hydrogen.

Professor David Knowles
CEO, The Henry Royce Institute

INTRODUCTION

The Henry Royce Institute is committed to the development of a strong UK hydrogen ecosystem. Royce is seeking materials-based solutions to key hydrogen challenges by delivering two multi-million pound investment programmes.

Royce has so far delivered over £5 million of funding to projects covering the breadth of the hydrogen supply chain with partners throughout the sector. This has been achieved through two investment activities, the Industrial Collaboration Programme (ICP) and Materials Challenge Accelerator Programme (MCAP), designed to tackle issues in the production, storage, distribution, use, and operational monitoring of hydrogen.

Since late 2022, Royce has funded a total of 43 projects through the two investment programmes. This has been made possible by the collaboration of 13 UK universities, 7 Research and Technology Organisations (RTOs) and 20 industry partners.

£5 MILLION OF FUNDING

13 UNIVERSITIES

43 PROJECTS

20 INDUSTRY PARTNERS

7 RESEARCH AND TECHNOLOGY ORGANISATIONS

ICP

ROYCE INDUSTRIAL COLLABORATION PROGRAMME

Through the Industrial Collaboration Programme, Royce is offering grant funding for research, development, and innovation sprint projects. Universities, research and technology organisations and companies can apply for funding up to total project costs of £125,000 for exploring innovative ideas with a focus on technology translation. By encouraging collaboration with industrial partners, the programme ensures that research is directly targeted at current, significant challenges faced by the hydrogen industry.

MCAP

ROYCE MATERIALS CHALLENGE ACCELERATOR PROGRAMME

The Materials Challenge Accelerator Programme provided short-term funding to progress priority areas for innovation identified in the Royce National Materials Challenge roadmaps and landscape documents. MCAP was open to all those working in higher education institutions, research technology organisations, and SMEs in the UK. Funding of up to £100,000 was available to support materials-related research and technology development with potential to deliver substantial impact to the UK hydrogen ecosystem.

THE HYDROGEN MATERIALS CHALLENGES

Royce has worked extensively with a wide range of stakeholders from across industry and academia to identify the major materials challenges that are preventing the establishment of a hydrogen economy.

The overriding challenges to widespread adoption and deployment of hydrogen were laid out in the 2021 report, 'Materials for end-to-end hydrogen'.

The report prioritised the five key research challenges which are crucial to the delivery of a functioning UK hydrogen ecosystem in line with 2050 net zero targets. Overcoming these will enable hydrogen to be produced, distributed, stored, used and monitored at scale to decarbonise a wide range of sectors.

HYDROGEN MATERIALS CHALLENGES

PRODUCTION	Materials-led solutions to radically improve performance, reduce cost, and extend operational lifetimes of green electrolysis routes.
STORAGE	Robust structural materials to enable large-scale hydrogen storage for fixed and mobile applications.
DISTRIBUTION	Materials capable of sustaining the thermal and mechanical strains associated with transporting hydrogen and purifying at point of use.
END-USE	Materials to withstand the full temperature range required for hydrogen use – from cryogenic liquid hydrogen to transport and fuel switching applications that operate at over 1,000°C.
OPERATIONAL MONITORING	Smart materials for real-time monitoring of critical infrastructure with the ability to report, mitigate or resolve problems before or as they arise.

Examples of particularly successful or innovative projects from both programmes – spanning the full hydrogen supply chain – are presented on the next few pages.

New and updated case studies for this edition are labelled.

CASE STUDY: ICP22

END-USE

Mechanical assessment of aerospace engine materials in hydrogen

ACADEMIC PARTNERS: CRANFIELD UNIVERSITY, UNIVERSITY OF MANCHESTER

INDUSTRY PARTNERS: ROLLS-ROYCE

The development of a hydrogen-fuelled gas turbine has been identified as a particularly key enabler for zero carbon emission flight, as gas turbine powered aircraft currently account for 96% of today's aviation carbon emissions. However, this will require a better understanding of the interaction of hydrogen with the materials used in engine construction.

This project demonstrated the capabilities of newly-upgraded hydrogen-fatigue testing facilities at Cranfield and explored the hydrogen embrittlement susceptibility of a stainless-steel alloy (SS347), which is often used in an aerospace environments.

The strength of the material was compared in air and hydrogen environments at room temperature and 200°C. Very little difference was found in the tensile strength of the alloy in these tests, suggesting it is relatively resistant to hydrogen embrittlement.

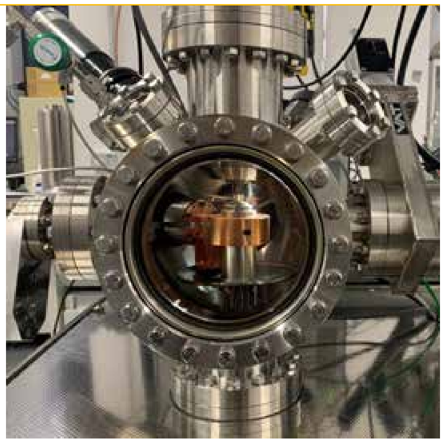
The follow-on programme resulting from this project (HOPTIMAL) will explore the impact of low temperature cycles (like those experienced during aircraft takeoff and landing) on the lifetime of the material.

"This work has been instrumental in the validation of new Royce facilities for materials certification in hydrogen, an area that is much needed within the UK and the larger community."

PROJECT IMPACT:

The upgraded Royce facilities were used to test and characterise stainless-steel in flowing pure hydrogen. This validated a new capability in hydrogen-fatigue testing and certification in UK research, which will contribute to the decarbonisation of aerospace.

This capability will be utilised in the new £14.8 million HYEST programme, funded by Innovate UK and the Aerospace Technology Institute.



CASE STUDY: ICP30

PRODUCTION

Applying in-situ transmission electron microscopy to optimise electrocatalysts for green hydrogen production

ACADEMIC PARTNERS: UNIVERSITY OF MANCHESTER, IMPERIAL COLLEGE LONDON

INDUSTRY PARTNERS: BP, INTERNATIONAL CENTRE FOR ADVANCED MATERIALS

This project was driven by a need to observe the operation and degradation of electrocatalysts in a liquid environment within a Transmission Electron Microscope (TEM). This will enable a deeper understanding of the materials processes which make green hydrogen production possible.

Examining the microscopic behaviour of in-situ electrolysers can provide insights into the catalyst's degradation in a real-world environment. Electrodes can behave differently in liquid environments compared to conventional lab testing setups. However, direct observation of this environment can be difficult.

To enable this, the team successfully deposited iridium on a working electrode inside a TEM electrochemical cell, then tested normal operation and cycling. Access to existing experimental setups, facilitated through Royce, provided a benchmark for comparison to the electrochemical cell being explored in this project.

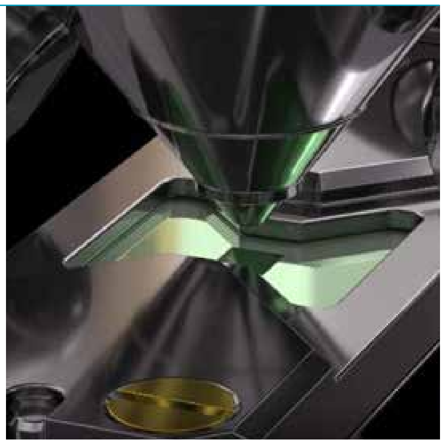
Beyond PEM electrolysers, the methodologies developed in this project can be applied more generally to other systems. For example, combining imaging and elementally sensitive techniques to study the evolution of copper catalysts during CO2 reduction, which is relevant to the £5 million bp-Johnson Matthey EPSRC Prosperity Partnership for developing new sustainable catalyst technologies.

"Collaborative discussions with the Royce project team (Manchester and Imperial) and other research groups were invaluable to help identify and guide electrode deposition and the specific research problems."

PROJECT IMPACT:

This project successfully benchmarked iridium oxide beam stability through in-situ testing. It uncovered a rich research area, which will be continued by a PhD student specifically recruited for this project.

In a major demonstration of this research project's impact, bp provided significant onward investment in the form of £2 million worth of equipment for investigating electrocatalysts using these techniques. The team has also received €3 million funding from the European Research Council for a consolidator project.



CASE STUDY: MCAP76 **UPDATED**

STORAGE

Properties of electroformed materials for hydrogen containment

INDUSTRY PARTNERS: ULTIMA FORMA LTD

The storage of hydrogen requires materials with low permeability and reduced susceptibility to hydrogen embrittlement. This project investigated the potential for electroforming metals to create lightweight hydrogen storage vessels which conform to any required shape.

Metals are significantly less permeable by hydrogen compared to polymers by an order of up to 10 million. However, they need to be continuous and strong to contain the pressurised gas. In electroforming, metals are deposited onto a plastic mandrel to create a seamless component which is thin, lightweight and resistant to high pressures.

These tanks are conformable to different shapes depending on the specialist application. This includes uses where electrification may not be viable – such as in large, hydrogen-powered vehicles or for hydrogen-powered aviation. Other potential future applications of this technology include the storage of cryohydrogen and of nuclear fusion materials.

In this project, electroformed materials were tested for hydrogen permeability and other mechanical properties required for hydrogen storage applications. The resulting data was distributed to key industry manufacturers and suppliers via the Royce Materials for Hydrogen Database.

"As a small company, we do not have the specialised testing facilities to generate the necessary materials property data. These facilities were made available by this grant at the Royce Institute at Manchester."

PROJECT IMPACT:

Ultima Forma has been successfully awarded a patent for the electroformed hydrogen barrier manufacturing process developed in this project.

They have used the technology developed in this project to demonstrate vacuum insulated liquid hydrogen pipe systems that both enclose the liquid hydrogen and maintain a vacuum jacket around it, extending the potential of this process to be used in future hydrogen transport systems.

CASE STUDY: ICP019

PRODUCTION

Novel tungsten carbide electrocatalysts for green hydrogen electrolysis

ACADEMIC PARTNERS: CRANFIELD UNIVERSITY, UNIVERSITY OF MANCHESTER

INDUSTRY PARTNERS: HARDIDE COATINGS

Scaling up production of green hydrogen will be constrained by pure water demand and the reliance on platinum-group metals as electrocatalysts. This project demonstrated the potential of using coated stainless steel plates to generate hydrogen from seawater.

A range of novel tungsten-carbide coatings were developed and applied by Hardide Coatings using the low temperature Chemical Vapour Deposition (CVD) process. These were subsequently characterised by the lab at Cranfield University, using a benchtop electrolyser setup created specifically for this project.

The coating offers both catalytic and protective properties to the substrate and can be applied to structures with complex shapes. CVD is a relatively mature technique used in the aerospace and oil and gas industries and can coat materials at a significantly larger scale than normally demonstrated in early-stage lab testing.

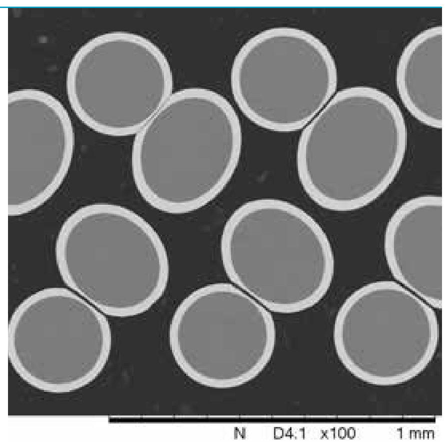
The SEM cross-section image below shows the Hardide coating as a light-coloured protective layer surrounding the steel mesh electrode wires. The coating performed well in this experiment, exhibiting catalytic activity comparable to pure platinum and producing 40% more hydrogen than standard titanium plates. They also remained stable and resisted degradation when tested in a saline solution for 100 hours, demonstrating their potential as catalysts for saltwater electrolysis.

"Royce at Cranfield provided the expertise and facilities in electrochemistry and materials characterisation critical for the success of this project."

PROJECT IMPACT:

This short project was instrumental in securing £550,000 follow-up funding from Innovate UK through the Resource Efficiency for Materials and Manufacturing collaborative R&D competition to test the efficiency and long-term stability of the coating.

Successful development of these coatings at an industrial scale will decrease the production costs of PEM electrolysers and reduce the dependency of the net-zero economy on critical minerals.



CASE STUDY: ICP305 UPDATED

MONITORING

Understanding degradation and predicting lifetime in solid oxide cells

ACADEMIC PARTNERS: IMPERIAL COLLEGE LONDON

INDUSTRY PARTNERS: CERES POWER

Solid oxide cell (SOC) electrolysis represents one of the most promising technologies for scalable green hydrogen production. To enable the rapid development of SOC technologies, an improved understanding of the electrochemical processes which impact electrode lifetimes is required.

This project was a continuation of an earlier ICP project, which explored the degradation of air electrodes in solid oxide cell electrolysers. Electron microscopy and photoelectron spectroscopy were used to determine the stability of the proprietary ceramic electrolysis cell developed and manufactured by UK-based Ceres Power.

These techniques enabled Ceres to investigate the interaction between the oxide layers in the SOC, and identify segregants and inhomogeneities on the sub-micron scale. These findings will provide critical insight into the stability of Ceres' cells and inform the lifetime modelling of the product – feeding into existing computational modelling tools.

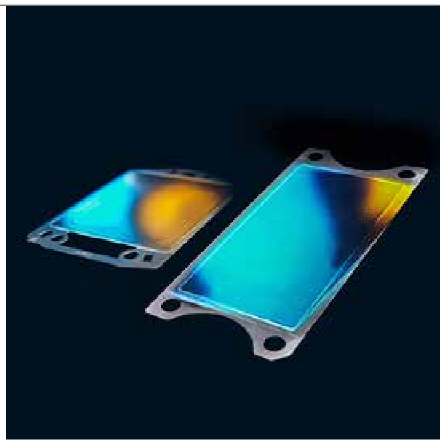
"New experimental capabilities were developed through this funding route that complements the cell development work that is possible within Ceres."

PROJECT IMPACT:

The monitoring work carried out in this project will enable an improvement in Ceres' next-generation cells – enhancing their resistance to degradation.

A better understanding of the electrochemical processes in the electrode allows improvements to be made without fundamentally altering the cell design or requiring the development of new materials.

Further collaborative funding has been secured by Ceres to continue their development of a detailed understating of SOC devices.



CASE STUDY: ICP332 **NEW**

END-USE

Damage tolerance of aerospace alloys at 20 kelvin

ACADEMIC PARTNERS: UNIVERSITY OF BRISTOL

INDUSTRY PARTNERS: ROLLS-ROYCE

When using liquid hydrogen as a fuel source, much of the system operates at the cryogenic temperatures where hydrogen is in liquid form. An in-depth understanding of material behaviour at these temperatures is required. This project studied the tensile strength and damage tolerance of a class of aerospace alloys at 20 kelvin.

The tensile strength and damage tolerance of 316L stainless steel and Hastelloy-X, a nickel based super alloy, were explored using a purpose-built cryogenic test rig at the Science and Technology Facilities Council's (STFC's) ISIS Neutron and Muon Source. Both materials were selected because of their widespread use within the aerospace industry.

The cyro tests determined the strength of the materials at cryogenic temperatures and found that for Hastelloy-X the ultimate tensile strength increased by 50% and the yield strength increased by 163% from its room temperature performance. Tests are now underway to determine the damage tolerance and crack resistance of these specimens.

"Thanks to this ICP we've been able to glean significant new information about the material properties of aerospace alloys at liquid hydrogen temperatures – information which is invaluable as we transition to a hydrogen driven society."

PROJECT IMPACT:

This project has furthered understanding about the mechanical behaviour of aerospace alloys at temperatures that would be experienced when operating liquid hydrogen-powered propulsion systems.

This research is continuing to be funded by Rolls-Royce, including a new PhD position, which will accelerate the transition to hydrogen as an aerospace fuel.

CASE STUDY: ICP323 **NEW**

PRODUCTION

Detecting production of hydrogen peroxide during electrolyser and fuel cell operation

ACADEMIC PARTNERS: IMPERIAL COLLEGE LONDON

INDUSTRY PARTNERS: JOHNSON MATTHEY

Hydrogen peroxide is a byproduct of the electrochemical reaction in the electrolysers that are key to green hydrogen production. The radicals formed from this hydrogen peroxide accelerate the degradation of electrolyser membranes, limiting their operational lifetime. This project developed a method for testing hydrogen peroxide levels.

There are both electrochemical and chemical mechanisms in electrolysers and fuel cells that generate hydrogen peroxide, and they are poorly understood. Imperial and Johnson Matthey developed a new approach to explore how the cathodes in fuel cells and electrolysers and the anodes in fuel cells create hydrogen peroxide in a mixed reaction environment where both hydrogen and oxygen are present.

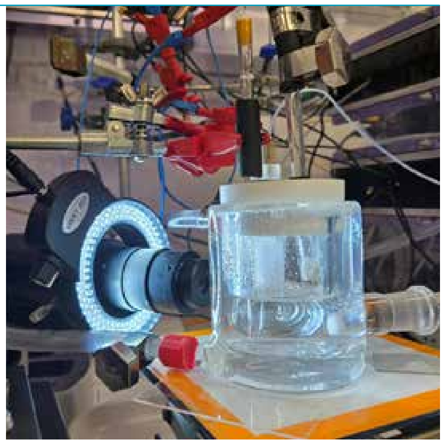
Current techniques for detecting hydrogen peroxide in electrolyser devices are time consuming and are subject to cross-sensitivity with the hydrogen also in the environment. This project successfully developed and demonstrated a technique that uses floating electrodes to test hydrogen peroxide production in the near real-world operating conditions of cathodes.

"This testing technique overcomes a serious bottleneck to screening future cathode candidates for reduced or even zero hydrogen peroxide production. It will unlock new technologies that mitigate this degradation pathway."

PROJECT IMPACT:

The hydrogen peroxide formation and reaction in catalysts can now be validated using this new monitoring device. It can be used without hydrogen interfering with the result and with improved sensitivity.

Johnson Matthey and Imperial's collaboration on this project has been so successful that Johnson Matthey have fully-funded a PhD to continue this research.



CASE STUDY: ICP348 **NEW** **PRODUCTION**

Novel 3D tomography reconstruction and modelling

ACADEMIC PARTNERS: UNIVERSITY OF SURREY, IMPERIAL COLLEGE LONDON

INDUSTRY PARTNERS: CERES POWER

The efficiency of Solid Oxide Electrolyser Cells (SOECs) is dependent on the microstructure of their electrodes. Conventional approaches to modelling these structure have relied on 2D imaging. This project has used machine learning to generate reliable 3D microstructure metrics to improve the efficiency of microstructure design.

Electrode microstructure porosity and phase connectivity play an essential role in the transport of gas, electrons and ions in the electrolyser cells. Understanding the detailed tomography of these structures supports the development of optimised solutions for cost-effective hydrogen production.

The software tool developed through this research generates 3D models of microstructures from 2D images using machine learning. Different properties like material fraction, porosity and structure are modelled.

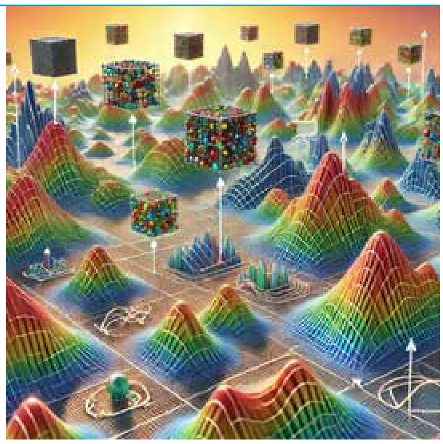
This research benefited from a combination of three key capabilities from its partners. Dr Qiong Cai's team at the University of Surrey completed the modelling, Ceres prototyped and tested different material compositions, and Dr Sam Cooper's team at Imperial developed the machine learning models.

"This project demonstrates that we can generate 3D microstructure information from 2D images using AI, reducing the need for resource-intensive imaging. It holds a lot of potential for cost-effective electrode design."

PROJECT IMPACT:

These modelling capabilities are a significant advancement in the efficiency and scalability of microstructure analysis for the design of the optimum microstructure for electrodes. Ceres and EPSRC have now funded a two-year post doc position in Dr Cai's team at the University of Surrey to continue this research.

Dr Cooper's team have spun-out a company, Polaron (www.polaron.ai), from Imperial. Polaron commercialises these capabilities and brings more efficient materials development to other sectors.



CASE STUDY: ICP329 NEW

END-USE

Hydrogen embrittlement testing methodology OPTIMisation for qualification of aerospace ALloys (HOPTIMAL)

ACADEMIC PARTNERS: CRANFIELD UNIVERSITY

INDUSTRY PARTNERS: DARVICK LTD, ROLLS-ROYCE, REACTION ENGINES

Hydrogen can be used in aerospace engines as a fuel source, but the compatibility of component metal alloys in these conditions must be verified. Whole lifetime testing at operating conditions would be time consuming, so accelerated testing capabilities have been developed.

This research involved three phases. In the first, a technique for quantifying the electrochemical charging and discharging of hydrogen was developed. Different geometries for the metal samples and electrolyte compositions were tested to determine a reliable method that shows potential for accurate, repeatable testing.

Secondly, Darvick designed and built a test rig. This has the capability to test the tensile strengths of samples with in-situ electrochemical charging. The rig can modify the charging method, charging type, loading regime (SSRT and fatigue), and temperature of a specimen.

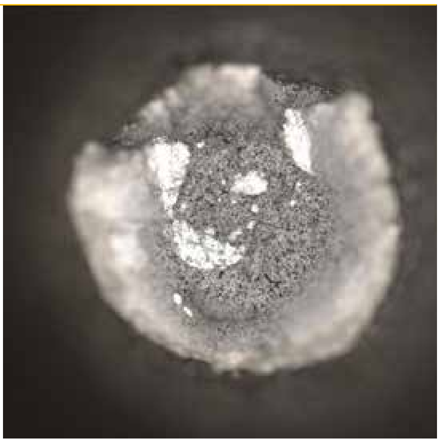
Finally, tests were run on samples of austenitic stainless steel to explore how different electrochemical and thermal charging techniques affected hydrogen embrittlement performance.

"Through this project, we have advanced our understanding and capability for testing materials in a hydrogen environment. This can be used to verify metal alloy performance in hydrogen engines."

PROJECT IMPACT:

Darvick is a SME business. Funding this research enabled them to design and build a new test rig, which offers a new capability in alloy sample testing in conditions that are of interest to hydrogen componentry.

Plans for testing of different alloys and of hydrogen permeation barrier coatings are already in place.



CASE STUDY: MCAP29

PRODUCTION

Designing stable supports to reduce the iridium loading in proton exchange membrane water electrolysers

ACADEMIC PARTNERS: IMPERIAL COLLEGE LONDON

INDUSTRY PARTNERS: TEER COATINGS

Iridium is a high-price, low-abundance material, the cost of which has increased by a factor of 10 in the last decade. It is often used in the production of hydrogen, but mining and extracting it is an extremely energy intensive process. Exploring alternative catalysts which are abundant and match iridium efficiency can future-proof hydrogen production.

Proton exchange membrane (PEM) electrolysis has been identified as one of the most promising green hydrogen production technologies. However, it currently relies on unsupported iridium to act as a catalyst and current collector. Iridium is a scarce material – more than 27 years of iridium production would be required to establish 1 TW of electrolyser capacity.

In this project, supports that can disperse iridium catalysts were developed to address this production bottleneck. The candidate material investigated for this project was niobium-doped titanium supports, which were created by Teer Coatings. This alteration was found to improve conductivity; however, it reduced the activity of the catalyst.

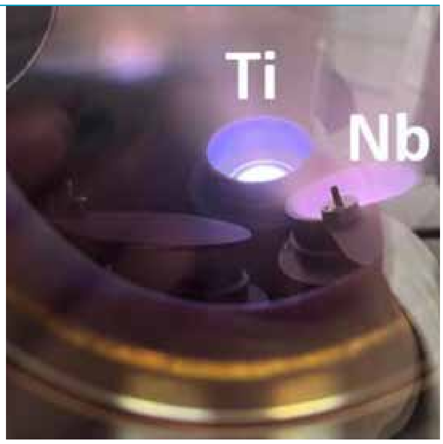
Through the collaboration with Royce, the research team was able to access highly accurate on-chip electrochemical mass spectrometry equipment which was used to characterise the effectiveness of the test materials.

"Taking advantage of the complementary expertise of Imperial College London and Teer Coatings, we have developed stable and conductive supports that enables significant reduction of iridium loading."

PROJECT IMPACT:

Stable and conductive supports that can disperse iridium-based catalysts were developed. These reduce the demand for iridium – a precious metal – in green hydrogen production.

Further research is planned as an extension to this project to optimise the size of the iridium oxide nanoparticles and enhance the activity and stability of the catalysts.



CASE STUDY: ICP3

DISTRIBUTION

Novel functional coating strategy for preventing hydrogen embrittlement in metals

ACADEMIC PARTNERS: UNIVERSITY OF OXFORD, UNIVERSITY OF SHEFFIELD

INDUSTRY PARTNERS: TWI

This project investigated a multi-functional coating solution for steel which mitigates hydrogen embrittlement. The process could allow existing gas distribution infrastructure to be repurposed for hydrogen.

Hydrogen can cause catastrophic failures to structural materials, reducing their strength and ductility through embrittlement. A Royce-funded collaboration between researchers at the Universities of Oxford and Sheffield and TWI demonstrated a new and effective coating solution that protects structural steels.

This collaboration drew on the specialist expertise of each partner: Oxford's strengths in laser-based manufacturing and mechanical characterisation, the University of Sheffield's experience of hydrogen characterisation, and TWI's industrial knowledge of processing and manufacturing.

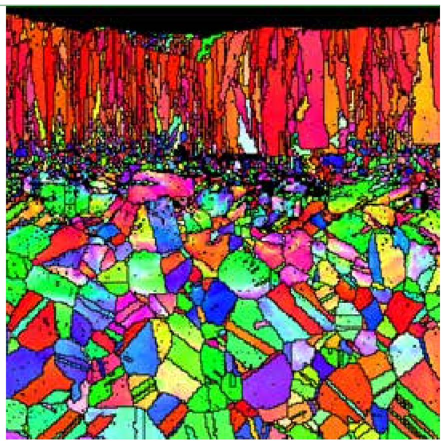
The novel coating is formed of two layers: a top coat that acts as a barrier to hydrogen, and a bond coat which readily absorbs any hydrogen that does manage to permeate the first layer. An extreme-high-speed laser application (EHLA) process was employed for this coating, which is significantly faster than other traditional methods.

"Royce has been instrumental in providing us with the necessary financial support, as well as the cutting-edge facilities that were critical in characterising hydrogen. More importantly, it facilitated a new fruitful collaboration with the three partners: Oxford, Sheffield and TWI."

PROJECT IMPACT:

The new coating was verified to be mechanically sound, scalable and decrease hydrogen permeation – which is the first direct proof-of-concept experiment of its kind.

This application technique shows great potential for unlocking the distribution of hydrogen through existing or new gas pipeline infrastructure. It would reduce the impact of hydrogen embrittlement, which at present accounts for a significant proportion of corrosion related failures costing £1.6 trillion each year.



CASE STUDY: MCAP49

MONITORING

Hydrogen diffusion and trapping in multi principal component alloys

ACADEMIC PARTNERS: UNIVERSITY OF WARWICK

Hydrogen embrittlement of stainless steels is poorly understood but significantly affects the usable lifetime of many industrial applications. Previous modelling work has either used very computationally-expensive methods or compromised on accuracy. MLIPs were used in this project to more efficiently model the diffusion of hydrogen.

Although they represent an interesting new area of research, MLIPs (Machine Learning Interatomic Potentials) can suffer from a complex and time-consuming training process. Hyper-Active Learning (HAL) is a new method for training these models which combats issues experienced by conventional machine learning tools: speed, computing cost and stability.

In this project, a simplified machine learning model was trained using HAL to simulate the interaction of a single hydrogen particle with nearby atoms. The process was demonstrated for the interaction of hydrogen with a group of 40 atoms and predicted the diffusion relatively well compared to existing models and empirical observation.

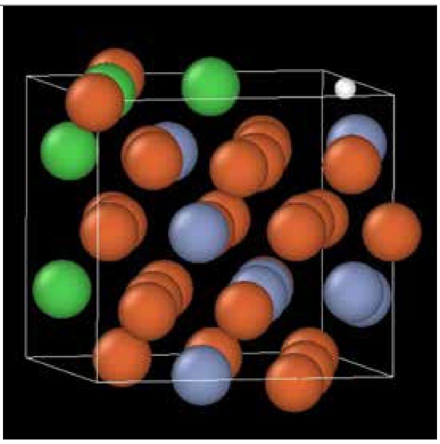
Future iterations of the model will involve a longer training process and adjustment of the initial parameters to improve accuracy and allow for the modelling of multiple hydrogen atoms.

"The machine learning methods used here are fully transferrable to other systems and we hope this work provides proof-of-principle for their adoption in industrial workflows for studying hydrogen embrittlement."

PROJECT IMPACT:

This pilot study has demonstrated that HAL-trained MLIPs can be an efficient and accurate way of understanding chemical processes without relying on conventional, computationally-expensive methods.

The project produced a MLIP that is capable of simulating stable molecular dynamics at elevated temperatures to improve understanding of hydrogen embrittlement. The methods used here are transferrable to other alloys and could be used to solve materials challenges across a wide range of industries.



CASE STUDY: ICP313 NEW

MONITORING

Spectroscopic studies of PEM electrolyser degradation

ACADEMIC PARTNERS: IMPERIAL COLLEGE LONDON

INDUSTRY PARTNERS: JOHNSON MATTHEY

Proton exchange membrane (PEM) electrolysers are the primary candidate for green hydrogen production, as their flexibility suits renewable energy production. Whilst their performance in model systems has been well studied, less is known about their performance in operational conditions.

PEM electrolyser catalysts contain iridium, a rare and finite element, which limits the scale-up potential of the technology. As such, there is a demand to understand more about their behaviour in order to optimise their performance.

Research has largely relied on model systems of catalysts to improve the performance of PEM electrolysers, but catalyst operation in actual device-relevant conditions remained to be studied. Using this ICP funding, a benchtop test system for PEM electrolysers was commissioned and installed. The researchers used this to test commercial catalysts in near real-world conditions and characterise their performance.

Crucially, these tests studied the catalysts in the presence of the ionomer, Nafion, fabricated as catalyst coated membranes. These identified that the degree of oxidation of the iridium catalysts in catalyst coated membranes is higher than model systems, suggesting that the ionomer layer can impact the PEM electrolyser performance and lifetime more than previously thought.

"This research enables study of catalyst performance under realistic device operating conditions that have not previously been explored, using a new state-of-the-art testing capability enabled by the funding from Royce."

PROJECT IMPACT:

This research enabled catalyst testing in PEM electrolysers under device-relevant operating conditions. It also uncovered the extent to which material performance varies between model laboratory-scale systems and catalyst coated membranes used in PEM electrolysers, which requires future research in order to scale PEM electrolysers and enable green hydrogen.

CASE STUDY: ICP023 **NEW** **END-USE**

Evaluating the cryogenic behaviour of austenitic materials for liquid-H_2 applications

ACADEMIC PARTNERS: UNIVERSITY OF MANCHESTER

INDUSTRY PARTNERS: JACOBS, AIRBUS

A cornerstone of Airbus's plan to deliver zero-emission (ZEROe) aircraft by 2035, is the development of liquid hydrogen (LH_2) fuel systems. A major challenge is to ensure the safe operation of these systems with the high duty cycle and long service life of commercial aircraft.

This project aimed to determine the mechanical properties of Invar 36, a potential material for hydrogen systems due to its low coefficient of thermal expansion (CTE), which decreases thermal stresses in critical components. Limited data exists on this low-CTE material and the impact of absorbed hydrogen at cryogenic temperatures.

The research established hydrogen charging and material testing protocols, exploring Invar 36's properties and microstructural stability down to -269°C. A stable microstructure and increased mechanical properties were identified at cryogenic temperatures. At -196°C, samples fractured outside hydrogen-charged areas, indicating that Invar 36 is not susceptible to typical hydrogen embrittlement.

"This work is paving the way for mechanical testing and hydrogen charging protocols in conditions relevant to hydrogen's use as an aerospace fuel, whilst encouraging open science and collaboration."

PROJECT IMPACT:

This novel study not only identified new material behaviours, but established a new testing procedure for Airbus to use on potential component materials, helping to ensure it remains a key played in the hydrogen economy.

The data generated from this testing could be used to develop science-based standards and guidance for innovative safety strategies for liquid and cryogenic hydrogen technologies and applications.

FULL PROJECT LIST

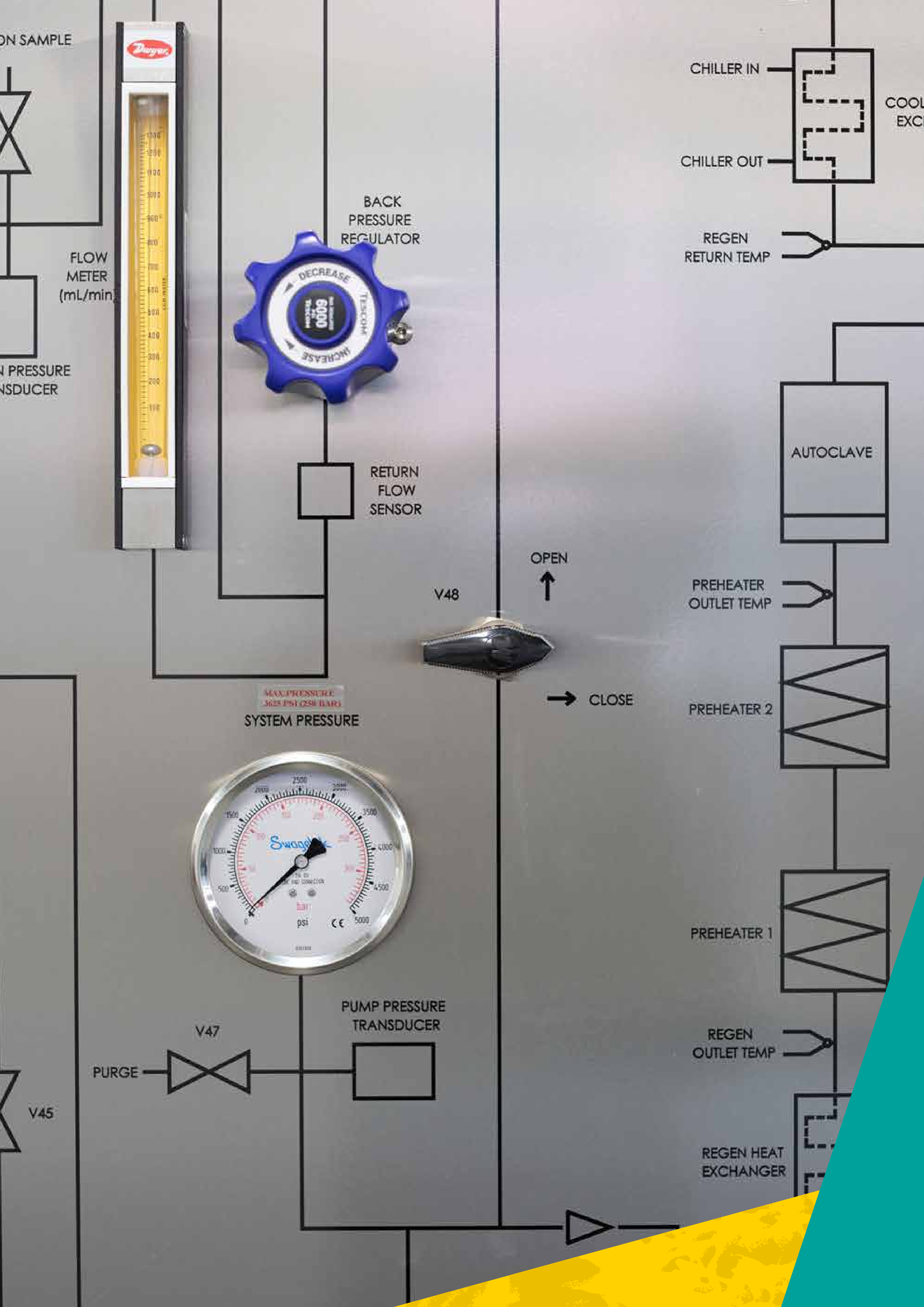
PRODUCTION

PROJECT DESCRIPTION	INDUSTRY PARTNERS	ACADEMIC PARTNERS
Establishment of electrochemical micro-test facilities for developing electrocatalysts for the generation of hydrogen	INEOS Electrochemical Solutions	University of Manchester
Novel tungsten carbide electrocatalysts for green hydrogen electrolysis	Hardide Coatings	Cranfield University University of Manchester
Applying in-situ transmission electron microscopy to optimise electrocatalysts for green hydrogen production	bp	University of Manchester Imperial College London
Designing stable supports to reduce the iridium loading in proton exchange membrane water electrolysers	Teer Coatings Ltd	Imperial College London
Reducing Iridium in proton exchange membrane electrolysers through catalyst and porous transport layers engineering	Johnson Matthey Mott Corporation	Manchester Metropolitan University Imperial College London
High-entropy alloy catalysts for green hydrogen production	Nikalyte	University of Oxford
High-throughput preparation of novel electrocatalyst for water splitting		University of Liverpool
Nanoparticle manufacture and operando studies under electrolysis		University of Oxford
Scale-up of PEM electrode deposition and testing		Imperial College London
Structural materials and meta-data for thermochemical electrolysis (METALYSIS)		Robert Gordon University
Understanding the effect of microstructural evolution of Solid Oxide Cell (SOC) electrode due to aging on real life operation in fuel cell and electrolysis for green hydrogen production	Ceres Power	University of Manchester
Advanced porous materials and processes for the next generation of Anion Exchange Membrane (AEM) electrolysers	Johnson Matthey	Coventry University
Detecting production of hydrogen peroxide during electrolyser and fuel cell operation	Johnson Matthey	Imperial College London
Electrocatalyst discovery to device: effective benchmarking for alkaline anion exchange membrane water electrolysis	Nikalyte Johnson Matthey	University of Oxford Manchester Metropolitan University NPL
Scale-up of novel earth-abundant electrocatalysts for sustainable green hydrogen production	INEOS Electrochemical Solutions	University College London
Novel 2D materials-based membranes for hydrogen crossover mitigation in water electrolyser	bp	University of Manchester
Material advancement for ultra-high efficiency, low-cost electrodes for high pressure electrolysis	Supercritical Solutions	Manufacturing Technology Centre National X-ray Computed Tomography
Novel 3D tomography reconstruction and modelling	Johnson Matthey	Imperial College London University of Surrey
Developing Resilient Catalysts For Low-grade Water Electrolysis	Ceres Power	Imperial College London

KEY – ORGANISATION TYPE: University Large enterprise SME RTO

	PROJECT DESCRIPTION	INDUSTRY PARTNERS	ACADEMIC PARTNERS
STORAGE	Capability development – cryogenic properties of H-charged metals	Airbus	University of Manchester
STORAGE	Gaseous hydrogen permeation test methodology to enable improved composites storage solutions for fuel cell vehicles		University of Manchester NPL Warwick Manufacturing Group
STORAGE	Properties of electroformed materials for hydrogen containment	Ultima Forma	
STORAGE	Multimodal, operando Raman and x-ray spectroscopies of electrochemical energy storage materials (MORSE)		University of Oxford NPL Diamond Light Source
DISTRIBUTION	Novel functional coating strategy for preventing hydrogen embrittlement in metals	TWI	University of Oxford University of Sheffield
DISTRIBUTION	Hydrogen adsorption & desorption		University of Manchester
DISTRIBUTION	Understanding hydrogen uptake in metals to safely deploy a hydrogen energy infrastructure		Imperial College London University of Manchester
DISTRIBUTION	Hydrogen Exposure Assessment of Real T-section Steel Welds (HEARTSWel)	Materials Processing Institute Liberty Pipes (Hartlepool) Ltd Natural Gas Transmission	University of Manchester University of Sheffield
END USE	Mechanical assessment of aerospace engine materials in hydrogen	Rolls-Royce	Cranfield University University of Manchester
END USE	Development of testing capability for materials under high water vapour content simulating hydrogen combustion in future engines (SAUNA)	Rolls-Royce Zircotec Ltd	Cranfield University Imperial College London
END USE	Development of hot isostatic pressed hydrogen-resistant A286 alloy towards net zero heat exchanger applications	Reaction Engines	University of Sheffield
END USE	High Entropy Alloy Coatings for Hydrogen Gas Turbines	Alloyed Ltd	University of Manchester
END USE	THERmal cycling of MAterials in water vapour Environments (THERMAE)	Rolls-Royce Zircotec Ltd	Cranfield University Imperial College London
END USE	Hydrogen embrittlement testing methodology OPTIMisation for qualification of aerospace ALloys (HOPTIMAL)	Darvick Ltd Rolls-Royce Reaction Engines	Cranfield University
END USE	Evaluating the cryogenic behaviour of austenitic materials for liquid-H2 applications	Jacobs Airbus	University of Manchester
END USE	Machine-learning based materials design of platinum-based alloys for hydrogen fuel cell cathodes	Johnson Matthey	University of Warwick
END USE	Novel low-cost hard-facing materials for hydrogen energy applications	Powderloop Technology Ltd	Manufacturing Technology Centre
END USE	Damage tolerance of aerospace alloys at 20 kelvin	Rolls-Royce	University of Bristol
MONITORING	Mechanistic understanding of solid oxide cell (SOC) electrode aging using multiscale characterisation	Ceres Power	University of Manchester
MONITORING	Investigation into the influence of material processing route on hydrogen-induced degradation	Manufacturing Technology Centre	University of Manchester
MONITORING	Understanding degradation and predicting lifetime in solid oxide cells	Ceres Power	Imperial College London
MONITORING	Spectroscopic studies of PEM electrolyser degradation	Johnson Matthey	Imperial College London
MONITORING	Hydrogen diffusion and trapping in multi principal component alloys		University of Warwick

KEY – ORGANISATION TYPE: University | Large enterprise | SME | RTO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TRANSDUCER
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V45
REGEN
OUTLET TEMP
REGEN HEAT
EXCHANGER

HENRY ROYCE INSTITUTE

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For further information contact:
info@royce.ac.uk

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February 2025