MATERIALS FOR THE ENERGY TRANSITION

MATERIALS FOR LOW-CARBON METHODS FOR GENERATION OF HYDROGEN AND OTHER RELATED ENERGY CARRIERS AND CHEMICAL FEEDSTOCKS

This publication forms part of the 'Materials for the Energy Transition' series. The Henry Royce Institute in collaboration with the Institute of Physics and the Institute for Manufacturing have convened the academic and industrial materials research communities to explore opportunities for materials to support the UK's net-zero by 2050 target.

HENRY ROYCE INSTITUTE

IOP Institute of Physics

IfM MANAGEMENT TECHNOLOGY POLICY

MATERIALS FOR THE ENERGY TRANSITION ROADMAP:

LOW-CARBON METHODS OF GENERATION OF HYDROGEN AND OTHER RELATED ENERGY CARRIERS AND CHEMICAL FEEDSTOCKS

SEPTEMBER 2020

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INTRODUCTION

The Challenge: Materials for the Energy Transition

Following release of the Committee on Climate Change (CCC) 2019 Report[1], the UK is committed to a new greenhouse gas emissions target: net-zero emissions by 2050.

The Executive Summary of the **2019 Committee on Climate Change Report** states:

"Delivery must progress with far greater urgency.

- ***2040 is too late for the phase-out of petrol and diesel cars and vans, and current plans for delivering this are too vague.***
- ***Over ten years after the Climate Change Act was passed, there is still no serious plan for decarbonising UK heating systems and no large-scale trials have begun for either heat pumps or hydrogen.***
- ***Carbon capture (usage) and storage, which is crucial to the delivery of zero GHG emissions and strategically important to the UK economy, is yet to get started. While global progress has also been slow, there are now 43 large-scale projects operating or under development around the world, but none in the UK.***
- ***However, falling costs for key technologies mean that the future will be different from the past: renewable power (e.g. solar, wind) is now as cheap as or cheaper than fossil fuels in most parts of the world."***

In response, the Henry Royce Institute (the Royce), in collaboration with the Institute of Physics (IOP), has engaged with academic and industrial materials research communities to explore solutions to the grand challenge of **"Materials for the Energy Transition"**. Through roadmapping workshops and associated community-led activities, technologies were identified where materials research can make a significant impact on greenhouse gas emissions.

The key drivers for this work have been (1) the pathways to net-zero emissions suggested in the CCC report, and (2) Royce-supported community workshops undertaken in 2019 to identify areas where investment in UK materials science can generate impact and contribute to the UK's energy transition. These included the "Atoms to Devices" workshop in Leeds (May 2019); the "Operando and In Situ Characterisation of Energy Materials" workshop at the Diamond Light Source in Harwell (July 2019); and, the "Multi-Modal Characterisation of Energy Materials" workshop in Cambridge (November 2019).

As a consequence, the following four areas were identified where materials science is critical to enabling a step-change in greenhouse gas reduction:

1. Materials for photovoltaic systems
2. Materials for low-carbon methods of hydrogen generation
3. Materials for decarbonisation of heating and cooling
    I. Thermoelectric energy conversion materials
    II. Caloric energy conversion materials
4. Materials for low loss electronics

[1] Committee on Climate Change Report: Net-Zero, January 2019, https://www.theccc.org.uk/publication/net-zero-the-uks-contribution-to-stopping-global-warming/

Materials Roadmaps

In 2020, the Royce together with the respective research communities explored the various materials challenges, targets, and timescales required to support the achievement of net-zero greenhouse emissions by 2050 of the four research areas outlined above. The CCC report and the related materials community engagement emphasised that these four areas are components of a broader ecosystem of materials technologies which together contribute to the UK's goals to deliver net zero by 2050. These roadmaps form the basis for bringing scientific research communities, industry and government together to address immediate and long-term requirements for the development of a suite of energy materials to replace fossil fuel-based energy technologies. The Royce collaborated with the Institute of Physics (IOP) to set out the programme of work and ensure community-wide feedback and engagement. Skills and expertise from the Institute for Manufacturing (IfM) were commissioned to ensure a robust roadmapping methodology, throughout the series of online roadmapping workshops, and to support community discussions.

Roadmap Objectives and Methodology

The main objectives for the five materials roadmaps at the outset were as follows:

- To understand the current state-of-art for each topic
- To define the most significant technical challenges for each area that are providing barriers to impact on net zero targets
- To define the anticipated future challenges for each area in contributing to net zero targets
- To identify solutions to these challenges that can make step-changes in delivery of technologies to contribute to net zero targets
- To identify the desired performance targets of such solutions

The methodology adopted was based on wide-ranging engagement with research communities to define the roadmap objectives and expectations, to design and customise the strategic framework for the roadmapping, to develop questionnaires for the research communities involved, and to modify workshop process steps to ensure participation of the entire research community. The workshops brought together academic and industrial experts in the four respective technology areas and involved both offline and online data collection phases. The offline phases were used for data collection from individual participants and publicly available research sources, followed by data consolidation and, where necessary and appropriate, prioritisation. The online workshops were used for data review, analysis and deeper exploration of essential issues. The quality and reliability of the process was maintained by a Steering Committee involving roadmapping facilitators and technical leads from each of the four research communities.

In total, 26 workshops sessions were held across the four technology areas between March 2020 and June 2020. These revealed several materials sub-topics of particular interest for contribution towards the net-zero targets, as well as highlighting important fundamental research and commercial technology enablers that need to be established. These outputs significantly aided research communities' understanding of the future direction of energy materials research, towards the achievement UK's net-zero emission targets by 2050.

Between March and June 2020, over 220 participants contributed to the creation of these five roadmaps from the UK academic and industrial materials communities. The outcomes are:

(1) an **executive summary** report, highlighting the main findings of the four roadmapping activities, published in July 2020;

(2) five **materials development roadmaps** towards net-zero emissions for 2050, published for research communities, funding bodies, government, policy-makers and industry leaders.

The five materials roadmaps generated are living documents, and Royce will engage with research communities regularly to review these documents and to develop further roadmaps as new materials systems and technologies emerge. We would like to thank all who have participated in these activities through the roadmapping workshops, interviews, surveys and research summaries.

Oversight of these community activities was through the “Materials for the Energy Transition” Steering Group: Professor Neil Alford, (Imperial College London), Professor Manish Chhowalla (University of Cambridge), Professor Richard Curry (University of Manchester), Professor Edmund Linfield (University of Leeds).

Programme management, reporting, and community engagement was undertaken by Royce and IOP: Mia Belfield (Royce), Ellie Copeland (IOP), Anne Crean (IOP), Isobel Hogg (IOP), Judith Holcroft (Royce), Professor David Knowles (Royce), Dr Amy Nommeots-Nomm (Royce), Dr Suman-Lata Sahonta (Royce), Professor Philip Withers (Royce), Dr Katharina Zeissler (Royce).

Roadmapping activities were coordinated by IfM: Dr Nicky Athanassopoulou, Dr Diana Khripko, Dr Imoh Ilevbare, Dr Arsalan Ghani, Andi Jones, Rob Munro.

Technical oversight of roadmaps was undertaken by Dr Oscar Cespedes (University of Leeds), Dr Katharina Zeissler (University of Leeds), Dr Oliver Fenwick (Queen Mary University of London), Dr Robert Hoye (Imperial College London), Dr Xavier Moya (University of Cambridge), Dr Ifan Stephens (Imperial College London), Dr Sam Stranks (University of Cambridge).

EXECUTIVE SUMMARY

The UK Government is committed to achieving net-zero greenhouse gas emissions by 2050. For this to occur, significant reductions in emissions by 2035 will need to be demonstrated. Only 11% of our energy supply is currently derived from renewables;[2] the remainder is largely derived from fossil fuels, resulting in colossal greenhouse gas emissions. The Committee on Climate Change has established that in order for the UK to decarbonise our energy supply and reach its net zero target, we need to increase our use of hydrogen by at least one order of magnitude. [3]

Hydrogen is an energy carrier, which is emission free at the point of consumption. There are four broad ways to produce hydrogen. The first route is from steam reforming, using either natural gas and steam, thermal methods or biomass gasification. Currently 95% of global hydrogen production is generated from fossil fuels,[4] *i.e. grey hydrogen,* producing large amounts of CO_2. *Blue hydrogen* is essentially grey hydrogen production coupled with CO_2 capture and storage. The second approach is electrolysis, which separates hydrogen from water using electricity in an electrolytic cell. The third method involves biological methods and predominantly uses microbes to convert biomass to hydrogen whilst the fourth method is direct photoelectrolysis which uses sunlight to split water into hydrogen and oxygen. These latter three methods of producing low carbon, *green hydrogen*, are not currently conducted at scale.[5]

The Henry Royce Institute is the UK's national institute for materials science research and innovation. Its research supports the government's industrial strategy to drive economic growth. The Royce brought together UK academic experts and industrial leaders from different research fields to explore different materials and methods that are required for the generation of hydrogen generation and other related energy carriers and chemical feedstocks at scale, using low carbon or zero carbon methods. The aims of this activity were to provide answers to the following questions:

- How can we enable hydrogen production technologies to be scalable to Terra Watt level through improved materials science and engineering approaches?
- What are the key fundamental and technological breakthroughs that would enable hydrogen production technologies to go beyond the efficiency and durability of current methods?
- Are other viable hydrogen generation options available (*e.g.* from waste biomatter)? How do these compare to steam reforming and electrolysis in terms of efficiencies, yields and scalability?
- Are there routes to improving efficiencies, reducing temperatures and capturing carbon from the steam reforming process so that its impact on greenhouse gas emissions can be minimised?
- How can improved materials enable the utilisation of hydrogen through other chemical carriers (*e.g.* ammonia)?

[2]Department for Business, Energy & Industrial Strategy, 'Aggregated energy balances showing proportion of renewables in supply and demand', 2019 https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/834155/Aggregated_Energy_Balances_2018__of_which_renewables_.pdf

3 HM Government. 'The Clean Growth Strategy' 2017 https://www.gov.uk/government/uploads/system/uploads/attachment_data/ file/651916/BEIS_The_Clean_Growth_online_12.10.17.pdf

4 The Royal Society 'Options for producing low-carbon hydrogen at scale, Policy briefing', 2018 https://royalsociety.org/~/media/policy/projects/hydrogen-production/energy-briefing-green-hydrogen.pdf

5 Committee on Climate Change, 2018 'Hydrogen in a low-carbon economy' https://www.theccc.org.uk/wp-content/uploads/2018/11/Hydrogen-in-a-low-carbon-economy.pdf

- What are the relevant targets that the materials, and materials–systems, need to demonstrate?

A key requirement for any technology development in this domain is demonstrate a **sustainable and stable resource supply,** as well as **end-of-life recycling**. For any existing or new materials used, improved recyclability and reactivation of materials will also be important for the sustainable, long-term use of these technologies.

The priority **topics** identified for enabling low-carbon methods of generation of hydrogen and other related fuels and chemicals that can make step-changes in research to reach 2050 targets were as follows:

- Proton exchange membrane water electrolysis electrolysers
  - Decrease or eliminate precious metals from catalysts
  - Improve cost, stability and conductivity of electrode materials
- Alkaline electrolysers
  - Improve membrane stability and conductivity
  - Improve catalyst activity
- Solid oxide electrolysers
  - Improve electrode and electrolyte materials
- Direct photoelectrolysis
  - More efficient and stable photoelectrode and photocatalyst materials
- Thermochemical synthesis of chemical feedstocks
  - More efficient catalysts and other materials that enable the production of chemical feedstocks at low pressures and temperatures
- Electrochemical reduction of carbon dioxide and nitrogen
  - Discover catalysts, electrodes and electrolytes yielding high activity and selectivity

We note that the latter two topics do not constitute methods to produce hydrogen, but rather pertain to the production of related chemical feedstocks or energy carriers. Nonetheless, there are many commonalities and between these topics and hydrogen production, both in terms of the underpinning science and the technological motivation.

The scope of our report does not include adjacent areas of materials science, relevant for the hydrogen value chain, such as (i) solid state hydrogen storage (ii) materials for fuel cells (iii) hydrogen embrittlement of hydrogen pipelines (iv) materials for hydrogen turbines. Nonetheless, the uptake of hydrogen at scale will require further research and development in these topics in the UK.

Some important **research and technology enablers** are required across all these topics for their successful development. These are:

- Community-wide bench-marking **testing protocols**;

- Testing facilities of new materials in prototype devices at single cell level using device geometries intermediate between those available in academic institutions and in full electrolyser stacks;
- **Materials production and processing capability** to produce novel devices for testing and evaluation;
- **Component development;** for example, durable and conductive alkaline membranes;
- Methods to improve the **recyclability and reactivation** of existing or new materials;
- Development of the fundamental understanding of **reaction and degradation mechanisms for accurate lifetime assessment, enhanced durability and end-of-life recycling;**
- **Ultra-sensitive analytical techniques**, which allow us to observe reaction intermediates, desired reaction products and undesired side products, including corrosion products, over the short time scales of typical laboratory experiments;
- Advanced ***operando* and *ex situ* characterisation (microscopy, spectroscopy, diffraction) techniques**, in partnership with UK National Facilities, strongly integrated with benchmark performance tests, to establish the characteristics of materials that are responsible for superior functionality;
- **Integrated experimental and computational programmes** where simulation tools both guide materials discovery and aid interrogation and interpretation of experimental data. For example, to predict new materials *in silico*, which is key to accelerating materials discovery;

In conjunction with the research developments, several **commercial and educational enablers** need to be established to accelerate the deployment and adoption of these technologies. These commercial enables are:

- The capability and funding to manufacture materials, catalysts and systems on a large scale so that they can be commercially tested. This could be achieved *via* integration with the **Catapult** network**.** Potentially, adventurous ARPA-type programmes for the UK in catalysis and energy materials.
- Access to **venture capital** and early **investment**, and global partnerships to make capital available **for small companies.**
- **British industrial champion(s)** that could drive forward the commercialisation of new technologies, as well as **hotspots of concentrated industry** that could be integrated with these technologies.
- **Well-resourced collaboration opportunities and support to such up relationships** within the UK between academia, industry, and research institutions, these could be facilitated with greater coordination and cooperation between the Henry Royce Institute, the UK Catalysis Hub, H2FC Supergen, the Faraday Institution, *etc*.
- Strong collaboration with **international** partners and integration in international supply chains.
- Participation in international research funding programmes *(e.g.* Horizon Europe's forthcoming Sunergy programme).

- Cheap **access to renewable electricity by** exploiting the UK's large off-shore renewable energy sources (RES). This could enable hydrogen integration with the electricity grid, as well as utilising the UK's manufacturing capability, but it will require **government support** and an **updated regulatory framework that reflects the opportunities for net-zero afforded by the hydrogen economy**. For example, **regulatory, political and/or tax incentives**, such as a carbon tax for wide roll-out of the use of renewable energies to enable 100% green hydrogen generation. This will offer the flexibility of being able to produce hydrogen in both a decentralised and centralised manner, at different scales and with distributed or non-distributed generation.
- **Regulation to accelerate industrial industries**, for example, green hydrogen use in refineries.
- A **business case** that differentiates the benefits of producing hydrogen through electrolysis using RES (green hydrogen) from hydrogen produced from fossil fuels (blue hydrogen).
- **Identification of niche markets** and **industrial processes** for the electrolytic production of hydrogen and other related fuels and chemicals. Capacity rather than availability is important for growth of the new sector

Education enablers include:

- **Improved and new training opportunities to fill the significant** UK **hydrogen skills gap**.
- **Training of new process engineers and electrochemical engineers** to design and operate large-scale operations.
- Updated university **curricula** that **raise awareness** of hydrogen and carbon-neutral fuels and feedstocks and the differences with the carbon positive equivalents used today
- **Alignment between universities and engineering bodies** (*e.g.* IChemE, IMechE, IEE, Energy Institute *etc*.) for university course accreditation schemes to promote and make attractive the uptake of these sustainable technologies.

These developments could collectively help to achieve efficient, durable and sustainable hydrogen production, which is scalable to the Tera Watt (TW) levels, suitable both for the UK and the rest of the world, with a net zero carbon footprint.

There is a significant opportunity within the country to invest in green hydrogen technologies in the UK to both exploit and support one of the largest renewable electricity generating capabilities in Western Europe. [6] For the UK to be able to capitalise on this opportunity, favourable government support is required in terms of progressive regulation frameworks and incentives for industry. Furthermore, because of the multidisciplinary nature of the field, integration of the different research activities and early engagement with industry are important for accelerating the commercialisation of technology. The generation of hydrogen and related chemical feedstocks is a multidisciplinary area that requires a variety of skills and knowledge, from modelling and surface science to process engineering to operate large-scale operations. It was suggested that this could potentially be achieved by forming an inclusive national network, including academia, central facilities, the Catapult network and industry partners, such as with apporpriate levels of funding.

[6] Department of Energy and Climate change 'UK renewable Energy Roadmap' 2011, https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/48128/2167-uk-renewable-energy-roadmap.pdf

An additional suggestion was the establishment of community-wide benchmarking testing protocols to synchronise and accelerate developments across the different academic groups and industry.

The **UK has numerous leading industries and academic researchers** in hydrogen and related energy carriers. [7] Further co-ordinated and targeted support would be both helping the UK's ambition to reach net zero by building a robust efficient, durable and sustainable hydrogen industry, and providing economic potential for exporting technology and know-how to the rest of the world.

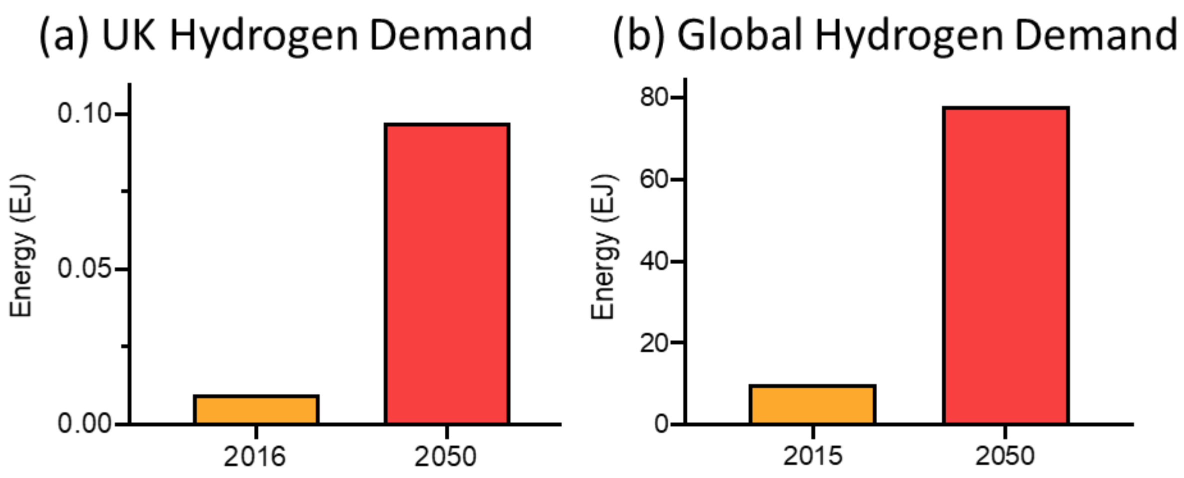
INDUSTRY / MARKET STATUS

The UK has become the first major economy in the world to pass a net zero emissions law. The ambitious target is to bring all greenhouse gas emissions to net zero by 2050, compared with the previous target of at least 80% reduction from 1990 levels.[8]

Currently in the UK, 11% of the total energy supply comes from renewables representing a distinct increase from previous years.[9] Most of the renewables comes from electricity derived from onshore and offshore wind, with the contribution of hydrogen currently being negligible.

Currently, 27 TWh per annum of hydrogen is produced in the UK, mainly *via* steam reforming using fossil fuels and only 1.1 TWh comes from water electrolysis.[10] It is anticipated that low-carbon hydrogen could be a significant contributor to renewable electricity generation by providing 30% of final energy consumption by 2050. If it is taken into consideration that 60-90 TWh per annum of low-carbon hydrogen could be generated from excess low-carbon power from offshore wind generation, this creates a unique opportunity for the UK to both utilise hydrogen technology to support its decarbonisation plans, and to become an energy exporter. [8]

The figure below highlights the use as of 2015 and predicted future demand for hydrogen in the UK and globally.



[7] Staffell, I., D. Scamman, A. Velazquez Abad, P. Balcombe, P. E. Dodds, P. Ekins, N. Shah & K. R. Ward (2019) The role of hydrogen and fuel cells in the global energy system. Energy & Environmental Science, 12, 463-491

[8] Department for Buisness, Energy, and Industrial Strategy, 'UK becomes first major economy to pass net zero emissions law' 2019 https://www.gov.uk/government/news/uk-becomes-first-major-economy-to-pass-net-zero-emissions-law

[9] Department for Buisness, Energy, and Industrial Strategy; Chapter 6; Renewable Sources of Energy' 2019 https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/840014/Chapter_6.pdf

[10] Committee on Climate Change, 2018 'Hydrogen in a low-carbon economy' https://www.theccc.org.uk/wp-content/uploads/2018/11/Hydrogen-in-a-low-carbon-economy.pdf

Figure 1: (a) Current and anticipated hydrogen demand for the UK[11], (b) Current and anticipated hydrogen demand worldwide, data from 2017. [12]

PROBLEM STATEMENT

Low-carbon hydrogen production at scale is expected to be an important contributor in the UK's decarbonisation strategy for 2050. One of the greatest barriers to producing green hydrogen is that it is not cost-competitive, especially for production at scale.[13]

Although some research has shown that the cost of green hydrogen is cost- competitive for niche applications, [14] the Committee on Climate Change[15] argued that, to enable low-cost production of green hydrogen, the cost for wind generation would need to fall to less than £10/MWh. Green hydrogen might be competitive in countries where solar power is very cheap. Other considerations for making low-carbon hydrogen commercially viable include power density, lifetime and balance of plant efficiencies.[16]

AIMS

There are specific research questions and challenges in each of the areas that need to be addressed to enable the development and adoption of existing or new materials that have the potential to make step-changes in research to reach UK 2050 targets. For hydrogen, the main questions that were investigated were:

- How can we enable hydrogen production technologies to be scalable to TW level through improved materials?
- What are the key fundamental and technological breakthroughs that would enable hydrogen production technologies to go beyond the efficiency and durability of current methods?
- Are other viable hydrogen generation options available (*e.g.* from waste biomatter)? How do these compare to steam reforming and electrolysis in terms of efficiencies, yields and scalability?
- Are there routes to improving efficiencies, reducing temperatures and capturing carbon from the steam reforming process so that its impact on greenhouse gas emissions can be minimised?
- How can improved materials enable the utilisation of hydrogen through other chemical carriers (*e.g*. ammonia)?
- What are the relevant targets that the materials and materials systems need to demonstrate?

[11] Committee on Climate Change, 'Net Zero Technical Report', 2019 https://www.theccc.org.uk/publication/net-zero-technical-report/
[12]Hydrogen Council, 'Hydrogen scaling up', 2017 https://hydrogencouncil.com/wp-content/uploads/2017/11/Hydrogen-scaling-up-Hydrogen-Council.pdf
[13] Staffell, I., D. *et al.,* The role of hydrogen and fuel cells in the global energy system. Energy & Environmental Science, 12, 2019, 463-491. https://doi.org/10.1039/C8EE01157E
[14] Staffell, I., D. Scamman, A. Velazquez Abad, P. Balcombe, P. E. Dodds, P. Ekins, N. Shah & K. R. Ward (2019) The role of hydrogen and fuel cells in the global energy system. Energy & Environmental Science, 12, 463-491
[15]Committee on Climate Change, 'Hydrogen in a low-carbon economy' 2018, https://www.theccc.org.uk/wp-content/uploads/2018/11/Hydrogen-in-a-low-carbon-economy.pdf
[16] The International Renewable Energy Agency 'Hydrogen from renewable power: Technology outlook for the energy transition' 2018 https://www.irena.org/-/media/Files/IRENA/Agency/Publication/2018/Sep/IRENA_Hydrogen_from_renewable_power_2018.pdf

The overall objective of this consultation was to develop a preliminary roadmap that can be used to guide discussions with the scientific and research communities, industry and government. Specifically, the materials research community and the Henry Royce Institute would like to:

- Understand the current state-of-the-art in each area of interest;
- Define in detail the key current challenges for each area that present barriers to meeting the UK's net zero targets;
- Define in detail the anticipated future challenges for each area that present barriers to meeting UK's net zero targets;
- Identify and prioritise the best topics to these challenges that can make step-changes in research to reach 2050 targets;
- Identify the desired performance targets of these topics.

A total of 55 participants attended the workshop and made high-value contributions to the content and discussions. There was good representation from both academia and industry. The full participant list is shown in Appendix I.

STRATEGIC RESEARCH OUTLOOK

The strategic landscape covers three time periods: the short-term (the next 5 years, *i.e*. up to 2025), the medium-term (the next 15 years, *i.e*. up to 2035) and the long-term (the next 30 years, *i.e*. up to 2050). It includes three broad layers: (1) challenges; (2) low-carbon methods of generation and other related chemical carriers; and (3) research, technology and enablers.

The second layer is subdivided into 10 sub-layers, as follows:

A. Low-temperature water electrolysis
B. High-temperature electrolysis and related systems
C. CO_2 utilisation
D. CO_2 storage
E. Direct photodriven processes
F. Hydrogen derived from bio-waste and renewable sources
G. Steam reforming
H. Integrated systems
I. Hydrogen storage and hydrogen carriers
J. Other

The third layer is sub-divided into seven sub-layers, as follows:

- Research and technology – Theoretical models
- Research and technology – Modelling and simulation
- Research and technology – *Operando* characterisation methods
- Research and technology – Reactor developments
- Research and technology – Integration
- Research and technology – Other
- Enablers – Infrastructure

In total, 16 challenges, 60 low-carbon methods of hydrogen generation and 25 research, technology and enablers were identified. The low carbon methods of hydrogen generation were prioritised further during the workshop. An overall strategic research outlook was synthesised for the Royce by bringing together the main challenges, low-carbon methods of hydrogen generation and research, technology and enablers, and by ensuring that the sequence of activities was logical and addressed all of the major challenges.

Figure 1 (below) shows the overall strategic research outlook for the low-carbon methods of hydrogen generation. The full list of challenges, low-carbon methods of hydrogen generation and research, technology and enablers are shown in Appendix V.

Strategic Landscape- Low carbon methods of hydrogen generation		Short-term 2020-2025	Medium-term 2025-2035	Long-term 2035-2050
Challenges	STEEPLE	Public perception and education		
		Hydrogen is not naturally occurring and takes huge amount of energy to release. A critical issue is where the electricity to undertake electrolysis would originate from.		
		Hydrogen is difficult to store and distribute.		
		There is need for grid scale storage solutions, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore significant materials innovation and systems integration are required.		
		The main production technologies that produced reasonable volumes of compressed hydrogen are not practically scalable, and thus it is essential that alternatives are found.		
		Industrial sector (reforming, ammonia, minerals, etc.)		Carbon-Neutral Aviation Fuel
		Viable technologies		
		Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point.		
		Subsidies to ensure competitiveness	Development of Carrier Distribution Network	
		UK wide H2 delivery network at appropriate H2 purity for maximum impact		
		Policy and regulation for hydrogen economy		
		Needs to be competitive in relation to Oil and Gas		
		Tax on fossil fuels		
		Understanding of legislation around renewables		

Topics	A. Low temperature water electrolysis	Establish stability of Pt catalysts in acid at PEM electrolyser at ultralow loading. Note that the amount of Pt required to drive hydrogen evolution in acid at PEM electrolysers cathodes is negligible, due to its exceptionally high activity. Hence the P Community data base and sharing best practices to increase performance. Standardisation for testing new catalytic materials and their performance	Develop proton conducting membranes that are impermeable to H2 and O2, have a high conductivity, high strength, high durability and ideally also cheaper than the current state of the art, based on Nafion. The development approach needs to be specified i Discover anode catalysts that function at pH 0 with 10 to 50 fold lower iridium content than current state of the art without compromising stability and minimise overpotential. Material recovery, recycling and circular thinking should also be considered. Currently in PEM electrolysers, the cost of the bimetallic plate and porous transport at the anode can exceed the catalyst, as it is challenging to find conducting materials that do not passivate. As such, precious metals are often used to minimise resist In order to lower the local bubble formation at the catalyst surface, design electrode/porous transport/catalyst layers in anode of electrolyser with a balance between hydrophobicity and hydrophilicity. The focus should be on technological solution on hi Scalability of production The study of fouling mechanisms by impurities in water and the development of remediation mechanisms and low grade water tolerant catalyst, membranes and electrolyser designs	Develop hydroxide conducting membranes that have equivalent conductivity, CO2 tolerance and stability to the current state of the art proton conducting membrane, Nafion (CO2 from air poisons alkaline membrane electrolysers). The operating parameters will Discover anode catalysts that function at pH 0 without precious metals, with same performance or better than current state of the art based on iridium. Discover anode catalysts that function in alkaline media, that minimise overpotential, without compromising stability.
	B. High temperature electrolysis and related systems	Integration of SOEC with fuel cells or (SOFC) and/or energy conversion devices such as gas turbines affords highly efficient large scale systems Develop small scale systems for local generation of hydrogen from PV or wind Design and manufacture of scalable SOEC systems capable of GW conversion of renewables High pressure operation to improve efficiency and initiate pressurization of resultant gas. Develop new materials-mechanical properties key	Solid oxide electrolysis producing hydrogen from steam typically works at 100% electrical to chemical efficiency at module level in commercial systems such as Haldor Topsoe or Sunfire. This equates to autothermal mode and has distinct advantages in terms Reduce reliance on critical elements such as cobalt and lanthanides to improve sustainability/cost Solid proton conducting oxide electrolysis has potential for lower temperature production of dry hydrogen and especially in process integration. Co-electrolysis of steam and CO2 provides syngas for chemical feedstock production and methanol or kerosene as transport fuels. Oxygen co-product from steam electrolysis offers benefit through integration with other processes.	
	C. CO2 utilisation		The big effort would be in coupling this process to renewable energy systems - thus if this is "carbon free" then the need to get lower temperatures, pressures is less important.	Electrochemical reduction using better electrode and catalytic materials. Methanol Synthesis/Conversion reactions. Stability for molecule catalysts, selectivity and limited materials are major challenges. Stability and efficiency is an issue for inorganic Need to develop CO2 utilisation technology to re-use the captured CO2 from steam-reforming of natural gas for H2 production. What can be done industrially in five years for minimizing greenhouse gas emissions is only CCUS. There is no shortage of CO2 at t
	E. Direct photodriven processes			Photocatalytic hydrogen synthesis through photoreforming of renewable / waste substrates, such as oxygenates, needs to be explored. Such substrates are easier to oxidise than water, with the potential for higher value oxidation products (e.g.: alcohols t Direct photoelectrochemical/photocatalytic water splitting is attracting extensive attention, with 100 m2 photocatalytic demonstration plants already operational in Japan. Cost projections suggest that with improved efficiency, some technologies could be
	F. Hydrogen derived from bio-waste and renewable sources		Structured catalysts combining microscopic design of catalysts structures (e.g. encapsulation of cheap transition metals) and macroscopic design of supports (e.g. optimisation of open-cell area-to-volume ratios) for steaming reforming of bio-waste and/or	
	G. Steam reforming	Partial Oxidation or other conventional processes for handling heavier hydrocarbons 100% carbon capture from SMR/ATR	The current process of methane steam reforming to produce hydrogen can meet the requirements of TW, depending on how much hydrogen is needed to produce in factory. High-temperature alloy materials for very large reactors may be the key. At present, the at	
	I. Hydrogen storage and hydrogen carriers	Examination of the materials properties of existing gas grid for suitability for high % levels of hydrogen. Materials challenges include: hydrogen leakage/safety, long-term durability	It is also important to think about sustainable synthesis of chemical feedstocks using H2 or directly through power to chemicals. Materials challenges include: new materials for solid oxide-based electrolysis for chemicals manufacture, catalysts for effic Ammonia is an excellent carbon-free hydrogen carrier or energy vector because it does not have storage problem and has mature large-scale synthesis (Haber-Bosch) and distribution	The reversible reaction from toluene to methyl-cyclohexane and back is another hydrogen carrier. The advantage is that these are benign materials that are readily available and can be safely recycled. It has also been investigated by Hrein in Japan and pr Multifunctional materials in hydrogen systems, e.g. whole system hydrogen storage from electrolyser to fuel cell without compressors and dehumidifiers/humidifiers. Materials challenges include: design of materials with tailored/flexible hydrogen storage A key challenge for getting to the TW scale is developing routes for international transport of large amounts of stored renewable energy from low-cost electricity regions in the form of chemical fuels synthesised sustainably, e.g. H2, CH4, methanol and am
	J. Other	Plasma decomposition of methane – interesting projects already Selective separation Hydrogen with natural gas		Thermocatalytic methane pyrolysis – trying to convert CH4 to a higher value carbon product – hydrogen is currently a by-product Thermochemical water splitting – requires high temperatures. Metal oxide cycling. Research currently in this area

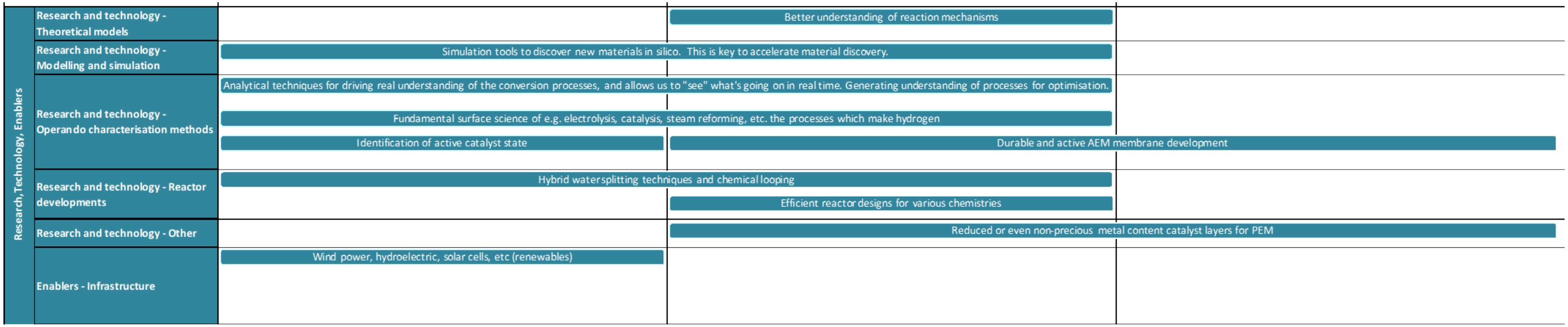


Figure 2: Strategic research outlook for energy materials for low-carbon methods of hydrogen generation (only prioritised items are shown)

Strategic Challenges - Low carbon methods for Hydrogen production	Short-term 2020-2025	Medium-term 2025-2035	Long-term 2035-2050
Challenges STEEPLE	Public perception and education		
	Hydrogen is not naturally occurring and takes huge amount of energy to release. A critical issue is where the electricity to undertake electrolysis would originate from.		
	Hydrogen is difficult to store and distribute.		
	There is need for grid scale storage solutions, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore significant materials innovation and systems integration are required.		
	The main production technologies that produced reasonable volumes of compressed hydrogen are not practically scalable, and thus it is essential that alternatives are found.		
	Industrial sector (reforming, ammonia, minerals, etc.)		Carbon-Neutral Aviation Fuel
	Viable technologies		
	Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point.		
	Subsidies to ensure competitiveness	Development of Carrier Distribution Network	
	UK wide H2 delivery network at appropriate H2 purity for maximum impact		
	Policy and regulation for hydrogen economy		
	Needs to be competitive in relation to Oil and Gas		
	Tax on fossil fuels		
	Understanding of legislation around renewables		

Figure 3a: Strategic challenges for energy materials for low carbon methods of hydrogen generation (only prioritised items are shown)

Strategic Research, Technology and Enablers - Low carbon methods for Hydrogen production	Short-term 2020-2025	Medium-term 2025-2035	Long-term 2035-2050
Research, Technology, Enablers: Research and technology - Theoretical models		Better understanding of reaction mechanisms	
Research and technology - Modelling and simulation	Simulation tools to discover new materials in silico. This is key to accelerate material discovery.		
Research and technology - Operando characterisation methods	Analytical techniques for driving real understanding of the conversion processes, and allows us to "see" what's going on in real time. Generating understanding of processes for optimisation.		
	Fundamental surface science of e.g. electrolysis, catalysis, steam reforming, etc. the processes which make hydrogen		
	Identification of active catalyst state	Durable and active AEM membrane development	
Research and technology - Reactor developments	Hybrid water splitting techniques and chemical looping		
		Efficient reactor designs for various chemistries	
Research and technology - Other		Reduced or even non-precious metal content catalyst layers for PEM	
Enablers - Infrastructure	Wind power, hydroelectric, solar cells, etc (renewables)		

Figure 4b: Strategic research, technology and enablers for energy materials for low carbon methods of hydrogen generation (only prioritised items are shown)

Topics				
	A. Low temperature water electrolysis	Establish stability of Pt catalysts in acid at PEM electrolyser at ultralow loading. Note that the amount of Pt required to drive hydrogen evolution in acid at PEM electrolysers cathodes is negligible, due to its exceptionally high activity. Hence the P Community data base and sharing best practices to increase performance. Standardisation for testing new catalytic materials and their performance	Develop proton conducting membranes that are impermeable to H2 and O2, have a high conductivity, high strength, high durability and ideally also cheaper than the current state of the art, based on Nafion. The development approach needs to be specified i Discover anode catalysts that function at pH 0 with 10 to 50 fold lower iridium content than current state of the art without compromising stability and minimise overpotential. Material recovery, recycling and circular thinking should also be considered. Currently in PEM electrolysers, the cost of the bimetallic plate and porous transport at the anode can exceed the catalyst, as it is challenging to find conducting materials that do not passivate. As such, precious metals are often used to minimise resist In order to lower the local bubble formation at the catalyst surface, design electrode/porous transport/catalyst layers in anode of electrolyser with a balance between hydrophobicity and hydrophilicity. The focus should be on technological solution on hi Scalability of production The study of fouling mechanisms by impurities in water and the development of remediation mechanisms and low grade water tolerant catalyst, membranes and electrolyser designs	Develop hydroxide conducting membranes that have equivalent conductivity, CO2 tolerance and stability to the current state of the art proton conducting membrane, Nafion (CO2 from air poisons alkaline membrane electrolysers). The operating parameters will Discover anode catalysts that function at pH 0 without precious metals, with same performance or better than current state of the art based on iridium. Discover anode catalysts that function in alkaline media, that minimise overpotential, without compromising stability.
	B. High temperature electrolysis and related systems	Integration of SOEC with fuel cells or (SOFC) and/or energy conversion devices such as gas turbines affords highly efficient large scale systems Develop small scale systems for local generation of hydrogen from PV or wind Design and manufacture of scalable SOEC systems capable of GW conversion of renewables High pressure operation to improve efficiency and initiate pressurization of resultant gas. Develop new materials-mechanical properties key	Solid oxide electrolysis producing hydrogen from steam typically works at 100% electrical to chemical efficiency at module level in commercial systems such as Haldor Topsoe or Sunfire. This equates to autothermal mode and has distinct advantages in terms Reduce reliance on critical elements such as cobalt and lanthanides to improve sustainability/cost Solid proton conducting oxide electrolysis has potential for lower temperature production of dry hydrogen and especially in process integration. Co-electrolysis of steam and CO2 provides syngas for chemical feedstock production and methanol or kerosene as transport fuels. Oxygen co-product from steam electrolysis offers benefit through integration with other processes.	
	C. CO2 utilisation		The big effort would be in coupling this process to renewable energy systems - thus if this is "carbon free" then the need to get lower temperatures, pressures is less important.	Electrochemical reduction using better electrode and catalytic materials. Methanol Synthesis/Conversion reactions. Stability for molecule catalysts, selectivity and limited materials are major challenges. Stability and efficiency is an issue for inorganic Need to develop CO2 utilisation technology to re-use the captured CO2 from steam-reforming of natural gas for H2 production. What can be done industrially in five years for minimizing greenhouse gas emissions is only CCUS. There is no shortage of CO2 at t
	E. Direct photodriven processes			Photocatalytic hydrogen synthesis through photoreforming of renewable / waste substrates, such as oxygenates, needs to be explored. Such substrates are easier to oxidise than water, with the potential for higher value oxidation products (e.g.: alcohols t Direct photoelectrochemical/photocatalytic water splitting is attracting extensive attention, with 100 m2 photocatalytic demonstration plants already operational in Japan. Cost projections suggest that with improved efficiency, some technologies could be
	F. Hydrogen derived from bio-waste and renewable sources		Structured catalysts combining microscopic design of catalysts structures (e.g. encapsulation of cheap transition metals) and macroscopic design of supports (e.g. optimisation of open-cell area-to-volume ratios) for steaming reforming of bio-waste and/or	
	G. Steam reforming	Partial Oxidation or other conventional processes for handling heavier hydrocarbons 100% carbon capture from SMR/ATR	The current process of methane steam reforming to produce hydrogen can meet the requirements of TW, depending on how much hydrogen is needed to produce in factory. High-temperature alloy materials for very large reactors may be the key. At present, the at	
	I. Hydrogen storage and hydrogen carriers	Examination of the materials properties of existing gas grid for suitability for high % levels of hydrogen. Materials challenges include: hydrogen leakage/safety, long-term durability	It is also important to think about sustainable synthesis of chemical feedstocks using H2 or directly through power to chemicals. Materials challenges include: new materials for solid oxide-based electrolysis for chemicals manufacture, catalysts for effic Ammonia is an excellent carbon-free hydrogen carrier or energy vector because it does not have storage problem and has mature large-scale synthesis (Haber-Bosch) and distribution systems. Need to develop materials for small scale and intermittent ammonia	The reversible reaction from toluene to methyl-cyclohexane and back is another hydrogen carrier. The advantage is that these are benign materials that are readily available and can be safely recycled. It has also been investigated by Hrein in Japan and pr Multifunctional materials in hydrogen systems, e.g. whole system hydrogen storage from electrolyser to fuel cell without compressors and dehumidifiers/humidifiers. Materials challenges include: design of materials with tailored/flexible hydrogen storage A key challenge for getting to the TW scale is developing routes for international transport of large amounts of stored renewable energy from low-cost electricity regions in the form of chemical fuels synthesised sustainably, e.g. H2, CH4, methanol and am
	J. Other	Plasma decomposition of methane – interesting projects already Selective separation Hydrogen with natural gas		Thermocatalytic methane pyrolysis – trying to convert CH4 to a higher value carbon product – hydrogen is currently a by-product Thermochemical water splitting – requires high temperatures. Metal

Figure 5c: Strategic topics for energy materials for low carbon methods of hydrogen generation (only prioritised items are shown)

DETAILED OUTPUTS

CURRENT STATE-OF-THE-ART

Methods for the production of hydrogen include thermochemical, biological, photochemical and electrolytic. Not all of these are low-carbon methods of hydrogen production. Depending on the feedstock and energy sources used for hydrogen production, these can be broadly grouped into the following four approaches: [17]

- **Steam reforming** of fossil fuels. This process typically uses natural gas and steam to generate "blue hydrogen" that is not low-carbon unless additional carbon capture and storage (CCS) processes are used in conjunction.
- **Electrolysis** that generates "green hydrogen" from water using electricity. This process can generate low-carbon hydrogen if renewable sources are used to provide the required electricity.
- **Direct photoelectrolysis,** where sunlight is harnessed and used directly to generate low-carbon hydrogen from water in a monolithic reactor or device.
- **Biological methods** that use microbes to convert biomass to hydrogen. These methods can potentially generate low-carbon hydrogen.

Figure 2 (below) summarises all the different methods for hydrogen generation.

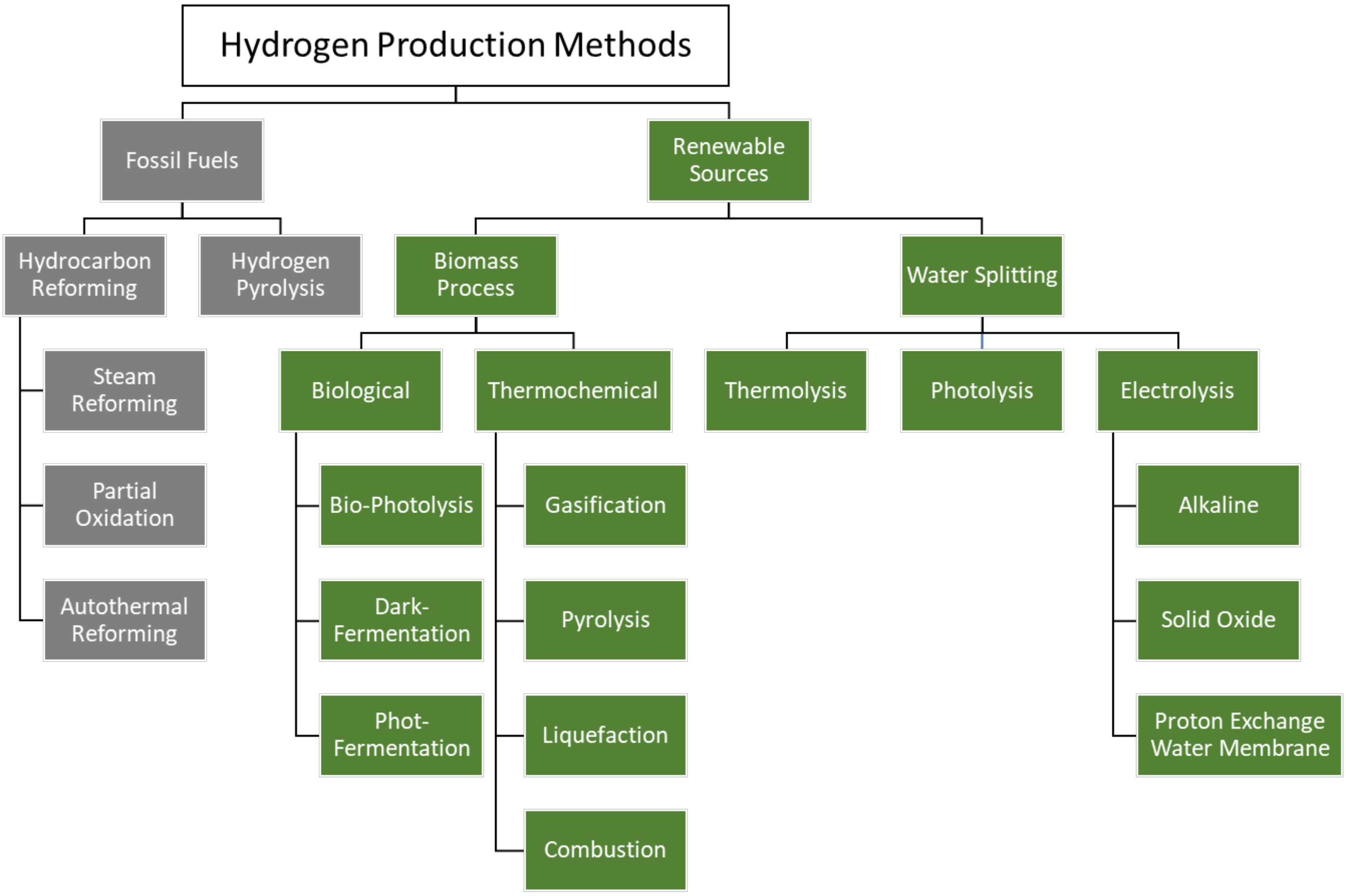


Figure 6: Different methods of hydrogen generation – adapted from Reference [18]

[17] The Royal Society 'Options for producing low-carbon hydrogen at scale, Policy briefing', 2018 https://royalsociety.org/~/media/policy/projects/hydrogen-production/energy-briefing-green-hydrogen.pdf

[18] Shiva-Kumar, S. & V. Himabindu 'Hydrogen production by PEM water electrolysis – A review'. Materials Science for Energy Technologies, 2, 2019, 442-454. https://doi.org/10.1016/j.mset.2019.03.002

While existing technologies such as steam reforming can make a useful contribution to hydrogen production in the short-term, step-changes will be needed in order to realise the dramatic increase to 2050 targets. Electrolytic approaches are highlighted as possibly offering the most significant potential for deployment in the near-medium-term.[5] The current state-of-the-art for all 10 areas that were considered in this work are summarised in the sections below.

A. Low-Temperature Water Electrolysis

Hydrogen production *via* water electrolysis follows a number of routes which (in decreasing technological maturity) are: a) Alkaline Water Electrolysis, b) Proton Exchange Membrane Electrolysis, c) High-temperature Solid Oxide Electrolysis, and d) Alkaline Exchange Membrane Electrolysis.[8] Methods (a), (b) and (d) are low-temperature processes operating below100^{o} C, whereas process (c) typically operates between 500 and 900 °C.

There are currently three different types of **low-temperature** water electrolysis technologies: Alkaline Water Electrolysis (AWE) (liquid electrolyte electrolysis), Anion Exchange Membrane Water Electrolysis (AEMWE) and Proton Exchange Membrane Water Electrolysis (PEMWE). These are all commercially available. Table 1 (below) shows the current state-of-the-art for each of these technologies.

Table 1: State-of-the-art for low-temperature water electrolysis technologies (adapted from references [19, 20,21,22])

Type	AWE	PEMWE	AEMWE
Electrolyte	KOH 20-40 wt.% in water	Proton exchange membrane	Anion exchange membrane
Electrode	Raney Ni mixed with, Fe, Co or, Mn at both electrodes	Anode: IrO_x on Ti Cathode: Pt/C,	Anode: Ni, NiO or Co Cathode: Pt or Ni
Current density	0.2 -0.5 A/cm^2	0.2 -3.0 A/cm^2	0.2 -0.8 A/cm^2
Temperature	40 -90 °C	20 -80 °C	40 -50 °C
Potential efficiency	73% LHV (i.e. at 1.7 V) at 0.3 A/cm^2	77% LHV (i.e. at 1.6 V) at 1 A/cm^2	63% LHV (i.e. at 2.10 V) at 1 A/cm^2
Pressure H_2 out	10 bar	10-200 bar	30 bar

AWEs use highly concentrated aqueous solutions of KOH as an electrolyte. They have been available commercially since the 19th century, and have been demonstrated up to the 100 MW scale. They have mostly been used to produce hydrogen for industrial purposes and are now being applied to make hydrogen for energy use, for example Nikola's H_2 truck refuelling stations in the USA will use NEL's alkaline electrolyser technology. Development over the last few decades has been minimal so there is considerable scope for new materials to improve AWE efficiency, which will be crucial to using this to produce hydrogen for energy applications efficiently. Generally, they have a lower CAPEX than other water electrolysis technologies.

[19] Tsotridis, G., *et al.* 'EU Harmonised Terminology for Low-Temperature Water Electrolysis for Energy Storage Applications' European Comission JRC Science for Policy Report, 2018. https://www.fch.europa.eu/sites/default/files/TERMINOLOGY_JRC_FINAL_GT.PDF

[20] Ayers, K., *et al.* 'Perspectives on Low-Temperature Electrolysis and Potential for Renewable Hydrogen at Scale' Annual Review of Chemical and Biomolecular Engineering 2019 10:1, 219-239 https://doi.org/10.1146/annurev-chembioeng-060718-030241

[21] Kotrel, S. & Bräuninger, S. in *Handbook of Heterogeneous Catalysis* (eds G. Ertl, H. Knoezinger, F. Schueth, & J. Weitkamp) 1936 (Wiley-CPH, 2008). ISBN: 978-3-527-31241-2

[22] Schmidt, O., 'Future cost and performance of water electrolysis: An expert elicitation study, International Journal of Hydrogen Energy' Volume 42, Issue 52, 2017,Pages 30470-30492, https://doi.org/10.1016/j.ijhydene.2017.10.045 .

PEMWEs use proton conducting polymeric membranes, mainly based on Nafion, which has a highly acidic pH. They have a higher CAPEX than AWEs, because of the electrode materials, electrolytes(membranes) and labour cost. The higher labour cost is a consequence of economies of scale. However, they hold several advantages over AWEs, namely (i) operation at high current densities at much greater efficiencies (see Table 2) (ii) the ability to work at fluctuating current densities, ideal for coupling with intermittent renewables, such as wind or solar (iii) the ability to produce pressurised H_2. PEMWEs are not as prevalent as AWEs, having only closed the technology readiness gap in recent years, but their uptake is set to increase strongly over coming decades. PEMWEs have been demonstrated up to the 10 MW level, [23] but there are plans to build much larger installations at a GW level by the mid-2020s e.g. ITM Power's planned Gigafactory in Sheffield. [24]

AEMWEs use an anion conducting solid polymer membrane as an electrolyte making a 'zero gap' device where the aqueous caustic electrolyte is removed or diluted. These should have many of the cost benefits of AWE but with higher efficiencies and current densities and be better at following loads and operate with pressure differential. These are generally considered to be pre-commercial. At least one start-up[25] company produces small scale systems ~5 kW and for the last 5 years there has been growing industry, research institute and academic interest - see for instance the three joint industry-research projects funded by FCHJU in 2019.[26] Laboratory scale devices have demonstrated performance similar to that of PEMWE electrolysis but the durability of materials is a major challenge. A key limitation has been the lack of suitable commercial anion exchange membranes (AEM). Both established manufacturers (EVONIK, TOKUAMA) and start-ups (IONOMER) based in Canada, USA, Germany, Japan and China are now developing these. The issue with many of these membranes is maintaining conductivity and chemical stability over 10,000s or even 100,000s of hours, dimensional stability, handling characteristics *etc*.

B. High-Temperature Electrolysis and Related Systems

A solid oxide electrolyser cell (SOEC) is an electrochemical conversion device that achieves the electrolysis of water (and/or carbon dioxide) using a solid oxide, or ceramic, electrolyte to produce hydrogen gas (and/or carbon monoxide) and oxygen. [27]
This electrolysis process normally operates at **high-temperatures** between 500 and 900 °C, so it typically achieves much higher efficiencies than can be achieved with low temperature electrolysis. Current state-of-the-art SOECs utilise a dense electrolyte, such as yttria-stabilised-zirconia (YSZ), fuel electrodes made out of a composite of nickel and YSZ, whereas a lanthanum strontium manganite –YSZ composite is used for the oxygen electrode. [28]

The technology is still in development, achieving 1,000 hours of operation at low current density with no evident degradation of the active components. Further advances in both materials and morphology are required to improve the durability of this technology so that it is stable for 100,000 hours .[10]

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[23] Dodds P. E., *et al. Opportunities for hydrogen and fuel cell technologies to contribute to clean growth in the UK.* H2FC SUPERGEN, London, UK, 2020, http://www.h2fcsupergen.com/wp-content/uploads/2020/04/H2FC-Infographic-Report-Summary-final.pdf

[24] Element Energy Limited, 'Gigastack Bulk Supply of Renewable Hydrogen Public Report' 2020 https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/866377/Phase_1_-_ITM_-_Gigastack.pdf

[25] www.enapter.com

[26] FCHJU AEMWE projects, https://cordis.europa.eu/project/rcn/226645/en ANIONE, https://cordis.europa.eu/project/id/875088 CHANNEL, https://cordis.europa.eu/project/id/875118 NEWELY

[27] Zheng, Y., *et al.* 'A review of high temperature co-electrolysis of H2O and CO2 to produce sustainable fuels using solid oxide electrolysis cells (SOECs): advanced materials and technology' Chem. Soc. Rev., 2017,46, 1427-1463, https://doi.org/10.1039/C6CS00403B

[28] https://www.sciencedirect.com/topics/engineering/high-temperature-electrolysis

E. Direct Photoelectrolysis

Currently, reports of efficient (>15%) solar power to hydrogen direct photoconversion[29] have been limited to high cost and/ or unstable materials and devices, with efficiencies for low cost and stable photoconversion devices being limited to circa 1%. The development of low cost, scalable and stable devices with efficiencies of 10–15% is needed so that photochemical routes can become commercially competitive. However, these approaches for production by water[30] splitting could be highly disruptive, and the UK is in a world leading position in this field. [31]
New approaches for direct hydrogen production by water splitting could be highly disruptive, and there are also has a number of ancillary benefits for example, most of the basic physical processes that underpin photochemical hydrogen production are also directly relevant to CO_2 reduction catalysts and photochemical routes that convert biomass to H_2 or other higher-value feedstocks (*e.g.*, new bioderived monomers for sustainable plastics). Photocatalytic methods are particularly attractive as means for deriving hydrogen and other high value chemicals, from low value feedstocks, such as polymer waste, biomass or glycerol. [32]

F. Hydrogen Derived from Biological Methods

Hydrogen production *via* biological methods is currently in its infancy and therefore provides a clear opportunity for higher-risk/higher-reward longer-term research activity. A particular challenge with , current biological methods, is that that are unable to sustain H_2 production for more than a few months, as the concomitant O_2 produced deactivates the active species. [33]

G. Steam Reforming

The methane steam reforming (MSR) technology is the oldest and most widely used route to converting CH_4 into H_2. The conventional process usually operates in a high temperature range of 973 -1173 K because of the highly endothermic nature of the reforming reaction. [34] Steam reforming of methane gas is used for almost 50% of the world's hydrogen production, with most other hydrogen obtained from other feedstocks, or by separation from natural gas. [35]

Steam reforming can be used with many different feedstocks, including methane, ethane, methanol, ethanol, acetone and higher hydrocarbons, and much research has been dedicated to characterisation of catalysts using these feedstocks. A great deal of attention has been focused on methane as a result of its favourable by-product formation compared to other feedstocks. [36]

Steam reforming of methane clearly has a role to play in the future of hydrogen production, because of the availability of natural gas and the extremely selective and active catalysts that are currently being produced. Advancements in catalyst preparation, composition, and reactor conditions, including microchannel reactors and membranes, allow larger than equilibrium values of hydrogen from a single reactor.[13]

[29] Cheng, W.H., *et al.* ' Monolithic Photoelectrochemical Device for Direct Water Splitting with 19% Efficiency' ACS Energy Letters 2018 3 (8), 1795-1800 DOI: 10.1021/acsenergylett.8b00920
[30] Takata, T., Jiang, J., Sakata, Y. et al. Photocatalytic water splitting with a quantum efficiency of almost unity. Nature 581, 411–414 (2020). https://doi.org/10.1038/s41586-020-2278-9
[31] https://www.nature.com/articles/s41929-018-0077-6?WT.feed_name=subjects_catalysis
[32] Achilleos, D.S., *et al.* Solar Reforming of Biomass with Homogeneous Carbon Dots. Angew. Chem. Int. Ed.. 2020, doi:10.1002/anie.202008217.
[33] Dubini, A., & Ghirardi, M. L., 'Engineering photosynthetic organisms for the production of biohydrogen' Photosynthesis research, *123*(3), 241–253 2015, https://doi.org/10.1007/s11120-014-9991-x
[34] Angeli, S.D., et al. 'State-of-the-art catalysts for CH4 steam reforming at low temperature' International Journal of Hydrogen Energy, Volume 39, Issue 5, 2014, 1979-1997 https://doi.org/10.1016/j.ijhydene.2013.12.001 .
[35] Lulianelli, A., *et al.* 'Advances on methane steam reforming to produce hydrogen through membrane reactors technology: A review', Catalysis Reviews, 58:1, 1-35, 2016 DOI: 10.1080/01614940.2015.1099882
[36] LeValley, T., *et al.* 'The progress in water gas shift and steam reforming hydrogen production technologies – A review', International Journal of Hydrogen Energy. 39. 2014 16983–17000. 10.1016/j.ijhydene.2014.08.041.

I. Hydrogen Storage and Hydrogen Carriers

Storing hydrogen, for example, in cars, requires high-pressure tanks or other storage materials systems, which present their own risks. The pressurisation is energy-intensive, and capacity is ultimately limited. For very large-scale storage of hydrogen (TWh scale), the most viable option is likely to be in geological formations such as salt caverns or depleted fossil fuel reservoirs. Salt caverns have been used to store hydrogen in the UK, but the economic and practical feasibility of each facility will need to be considered in more detail.

Today a large part of hydrogen is used to produce chemical feedstocks such as ammonia -NH_3 and methanol CH_3OH using thermochemical processes at high-temperatures and pressures; the hydrogen is derived from steam reformed methane. As CO_2 is captured in large amounts, compounds such as methanol, and C_2 products such as ethanol could be produced, possibly on a localised basis, by thermal CO_2 reduction using electrolytic green hydrogen. A similar case could be made for using electrolytic H_2 for sustainable NH_3synthesis *via* the Haber Bosch process. However, several scientific and technical challenges need to be overcome in order for these processes to compete with current methods. Indeed, chemicals such as $NH_3$and CH_3OH are also highly attractive as solar fuels.

The need to separately produce electrolytic H_2 could be circumvented by the direct electrochemical reduction of N_2 to NH_3 or CO_2 to hydrocarbon and oxygenates. Even so, direct CO_2 and N_2 reduction are still in their infancy and significant fundamental research and discovery is required.

CURRENT CHALLENGES

Overall, 16 challenges were identified by the participants, which have, or may have, an impact on the development and implementation of materials for low-carbon methods of hydrogen generation. The direct, *unedited*, outputs of the survey are shown in Table 2 (below).

Table 2: Main current challenges for energy materials for low-carbon methods of hydrogen generation

	Challenges	Timescale
C1	Public perception and education	ST
C2	Hydrogen is not naturally occurring and takes a huge amount of energy to release. A critical issue is where the electricity to undertake electrolysis would originate from.	ST-MT
C3	Hydrogen is difficult to store and distribute.	ST-MT
C4	There is a need for grid-scale storage topics, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore, significant materials innovation and systems integration are required.	ST-MT
C5	The main production technologies that have produced reasonable volumes of compressed hydrogen are not practically scalable, and thus it is essential that alternatives are found.	ST-LT
C6	Industrial sector (reforming, ammonia, minerals, *etc.*).	ST-MT
C7	Carbon-neutral aviation fuel.	LT
C8	Viable technologies.	ST-MT
C09	Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing a low-carbon hydrogen infrastructure from source to delivery point.	ST-MT
C10	Development of a Carrier Distribution Network.	MT
C11	Subsidies to ensure competitiveness.	ST
C12	UK wide H_2 delivery network at appropriate H_2 purity for maximum impact.	ST-MT
C13	Policy and regulation for hydrogen economy.	ST-MT
C14	Needs to be competitive in relation to oil and gas.	ST-MT
C15	Tax on fossil fuels.	ST-MT
C16	Understanding of legislation around renewables.	ST-MT

PROPOSED TOPICS FOR LOW-CARBON METHODS OF HYDROGEN GENERATION

Overall, 60 potential **topics** were identified for materials for low-carbon methods of hydrogen generation. These were subdivided into 10 sub-layers, as shown in Table 3 (below).

Table 3: Number of low-carbon methods of hydrogen generation identified for different sub-layers

Sub-layers	Number of topics proposed
A. Low-temperature water electrolysis	11
B. High-temperature electrolysis and related systems	8
C. CO_2 utilisation	5
D. CO_2 storage	3
E. Direct photodriven processes	5
F. Hydrogen derived from bio-waste and renewable sources	4
G. Steam reforming	6
H. Integrated systems	4
I. Hydrogen storage and hydrogen carriers	5
J. Other	7

There was, overall, a good balance of topics proposed across all the sub-layers, with only sub-layers *D. CO_2 storage*, *F. Hydrogen derived from bio-waste and renewable sources* and *H. Integrated systems* having fewer topics. There was a good balance between short-, medium- and long-term topics.

Each of the 60 topics proposed during the workshop were assessed using two different and broadly separate considerations: reward and feasibility. Reward was broadly defined as the magnitude of the opportunity plausibly available for scalability and decreasing the UK's carbon footprint. Feasibility was broadly defined as how well prepared the opportunity could be for industrial applications in terms of efficiency, sustainability, durability, integration, use of renewable sources, and use of existing infrastructure.

The specific reward and feasibility criteria had been selected prior to the workshop by the Royce and are shown in Table 4 (below).

Table 4: Reward and feasibility criteria used to assess the different topics for low carbon methods of hydrogen generation

Reward
Is the technology scalable to the TW level, for example, is it constrained by the supply of raw inputs, *e.g.* fossil fuels, waste biomatter?
To what extent would this technology decrease the carbon footprint within the UK?
Even if it is not scalable to the TW level, or the carbon footprint is significant, would the increased adoption of this technology enable the wider uptake of hydrogen in the short-term?
Feasibility
Does the technology have the potential to be sufficiently efficient or durable for industrial applications?
Does the technology have the potential to sustain sufficiently high hydrogen production rates for industrial applications?
Is the technology amenable to integration with renewable energy sources (e.g. intermittent operation)?
Is the technology amenable to integration with current infrastructure?

The topics were divided into short-, medium- and long- term lists. Each list contained an approximately similar number of topics. 18, 25 and 17, respectively. Every participant was asked to select FOUR priority topics from each list based on the reward and feasibility criteria.

The selection process took place in two parts. First, each participant was asked to review the topics in each short-, medium- or long- term lists and independently choose four, based on the three reward factors. In the second step, participants were asked to consider only the four topics they had already selected, and to choose two topics that had the best feasibility potential based on the four feasibility factors. The second step narrowed the topics down to a shorter list of 36, which were considered further during the workshop. This shorter list still contained topics from all sub-layers of the roadmap. The prioritised topics are shown in Figure 7-9 (below) for the short, medium and long terms, respectively. The topics highlighted in **bold** were selected for further exploration.

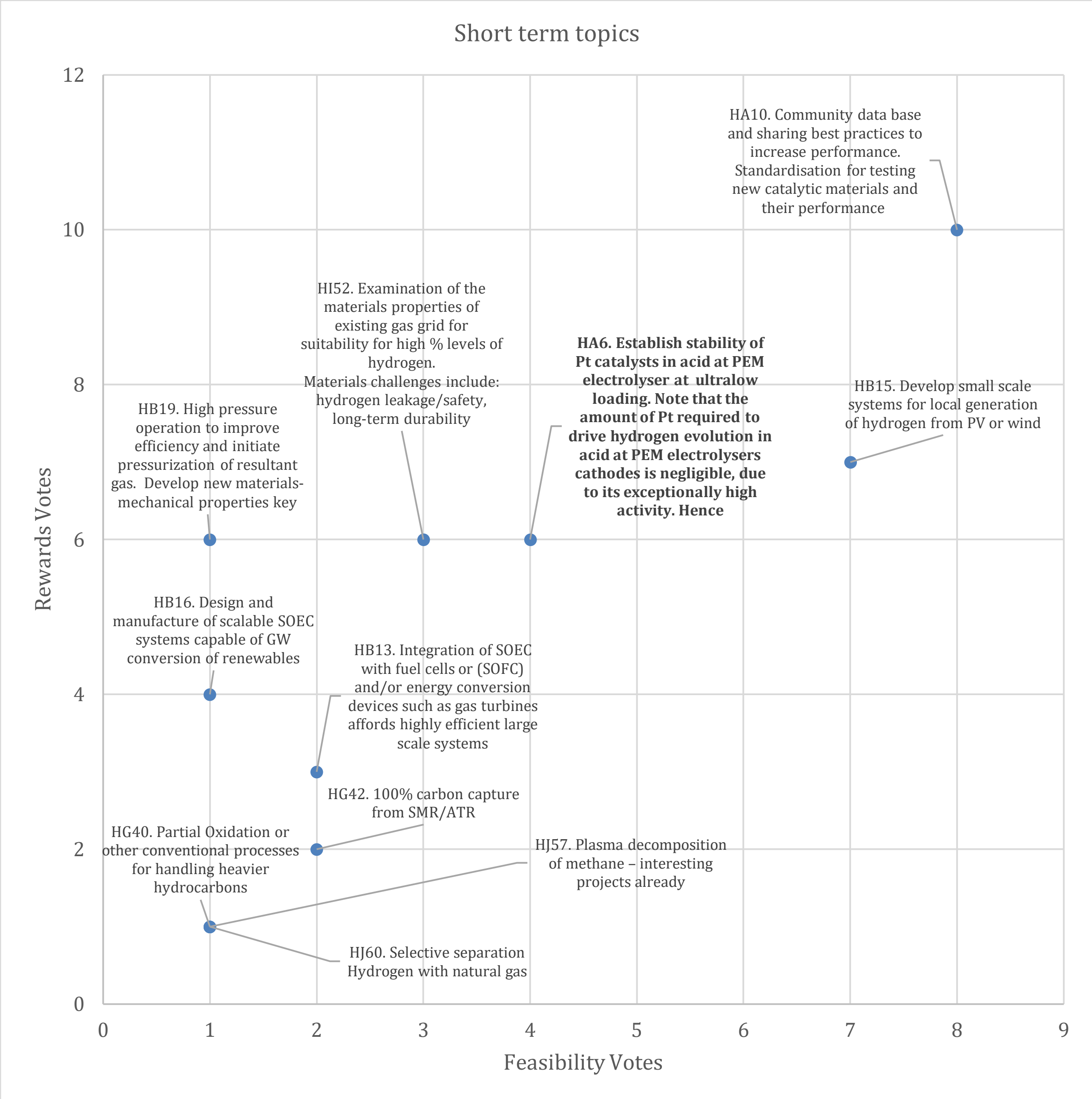

Figure 7: Topic prioritisation chart for the short-term using feasibility–reward axis. Topics highlighted in **bold** were selected for further exploration

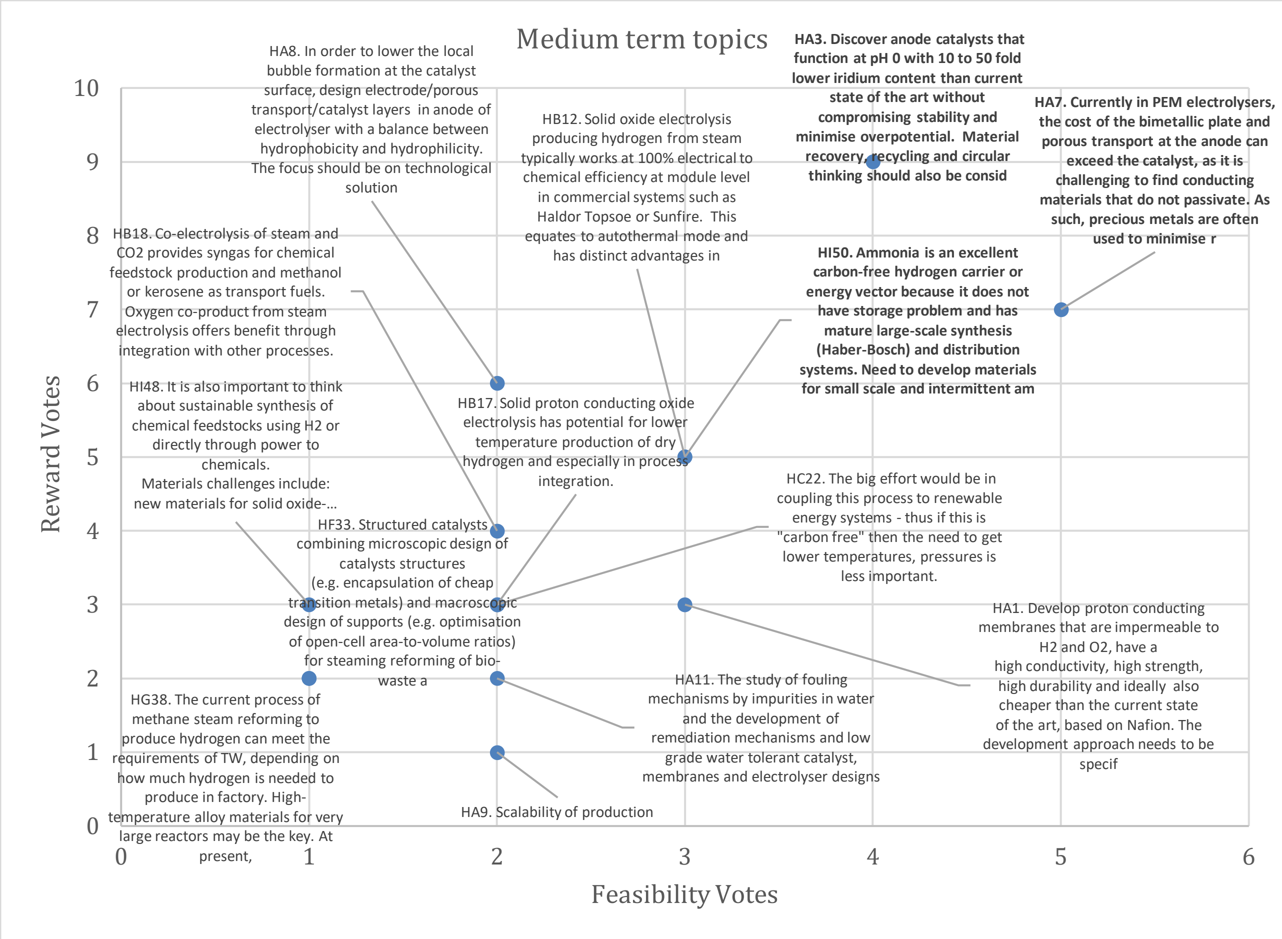

Figure 8: Topic prioritisation chart for the medium-term using feasibility–reward axis. Topics highlighted in **bold** were selected for further exploration

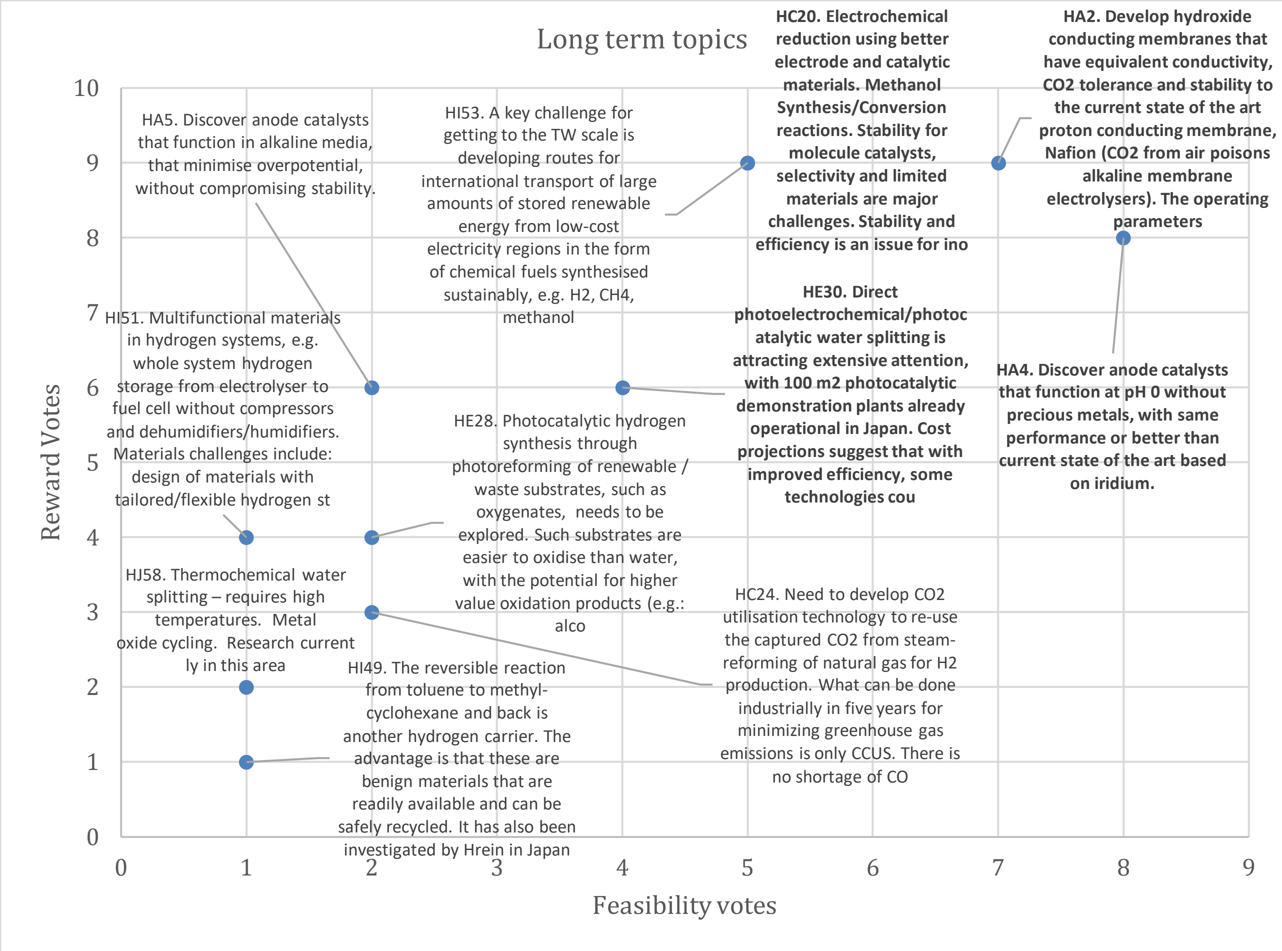

Figure 9: Topic prioritisation chart for the long-term using feasibility–reward axis. Topics highlighted in **bold** were selected for further exploration

Topics placed on the top-right quadrant (high feasibility and high opportunity) were of immediate interest. Topics on the top-left quadrant (low feasibility / high opportunity) may represent possible long-term opportunities. Topics placed on the bottom quadrants (low / high feasibility and low opportunity) were not automatically dismissed, as they might enable other topics or support longer-term prospects.

Most topics voted for were from the sub-layers of *A. Low-temperature water electrolysis, B. High-temperature electrolysis and related systems* and *I. Hydrogen storage and hydrogen carriers*, as shown in the figure below. Some sub-layers had no votes for the topics listed, such as *D. CO_2 storage* and *H. Integrated systems* (See Figure 10).

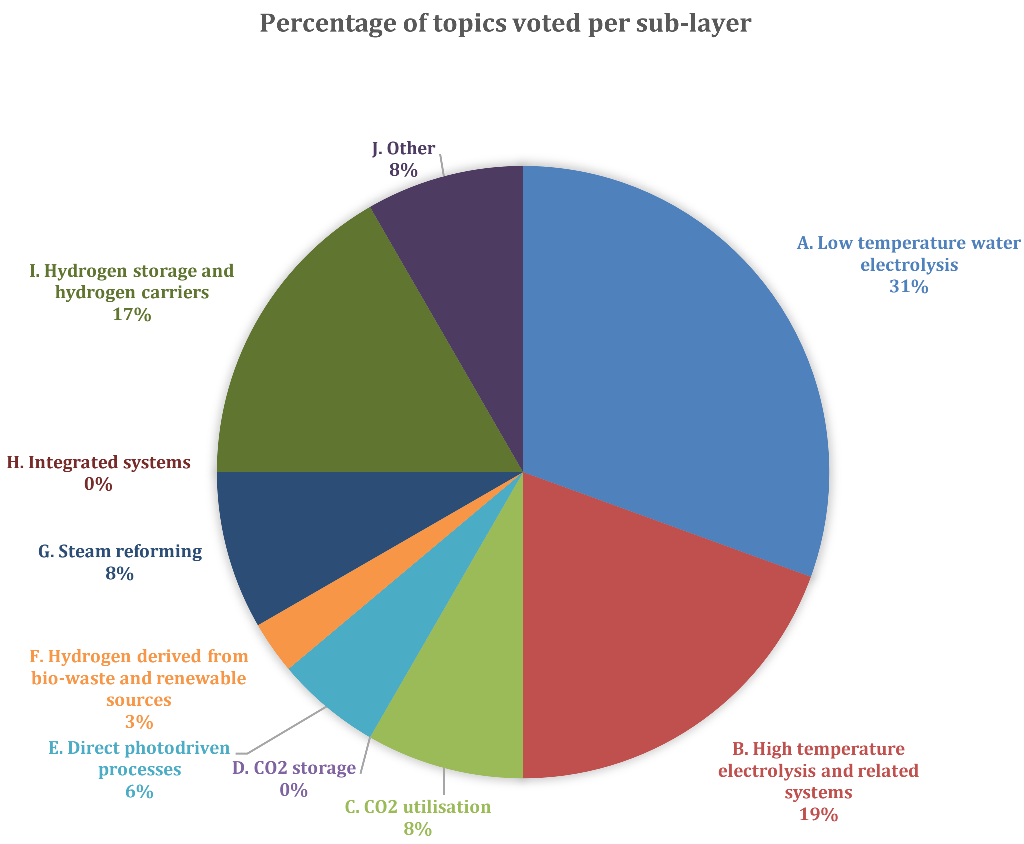

Figure 10: Percentage of topics voted per sub-layer

Some topics were further grouped, as they were quite similar. These were:

- HA3 and HA4
- Sustainable synthesis of chemical feedstocks using H_2 or directly through power to chemicals (HI48, HI50 and HI53)

In order to achieve a balanced selection, topics and groups were then reviewed regarding the following aspects: their relative scores and position in the 2x2 chart; the sub-layers to which they belonged; and the timeline of the application (short-, medium- or long-term).

Consequently, the following six topics were shortlisted for further exploration:

- Proton Exchange Membrane Water Electrolysis electrolysers
    - Decrease or eliminate precious metals from catalysts
    - Improve cost, stability and conductivity of electrode materials
- Alkaline electrolysers
    - Improve membrane stability and conductivity
    - Improve catalyst activity
- Solid oxide electrolysers
    - Improve electrode and electrolyte materials
- Direct photoelectrolysis

    - More efficient and stable photoelectrode and photocatalyst materials
- Thermochemical synthesis of chemical feedstocks
    - More efficient catalysts and other materials that enable the production of chemical feedstocks at low pressures and temperatures
- Electrochemical reduction of carbon dioxide and nitrogen
    - Discover catalysts, electrodes and electrolytes yielding high activity and selectivity

The descriptions and roadmaps for shortlisted topics are described in the following sections. The full list of topics and the votes they received are shown in Appendix IV.

PRIORITY TOPICS

Six topics were selected for further discussion and exploration in small groups of four to seven participants. These projects were:

- Proton Exchange Membrane Water electrolysers
  - Decrease or eliminate precious metals from catalysts
  - Improve cost, stability and conductivity of electrode materials
- Alkaline electrolysers
  - Improve membrane stability and conductivity
  - Improve catalyst activity
- Solid oxide electrolysers
  - Improve electrode and electrolyte materials
- Direct photoelectrolysis
  - More efficient and stable photoelectrode and photocatalyst materials
- Thermochemical synthesis of chemical feedstocks
  - More efficient catalysts and other materials that enable the production of chemical feedstocks at low pressures and temperatures
- Electrochemical reduction of carbon dioxide and nitrogen
  - Discover catalysts, electrodes and electrolytes yielding high activity and selectivity

High-level roadmaps for each of the six topics are described in the next sections. The topic roadmaps include the following fields:

- A detailed description, including the ideal end-state;
- The scope and boundaries of the solution, indicating aspects that are included and excluded from further development;
- The impact that the solution is expected to have on the UK 2050 decarbonisation targets;
- Key technological goals in the short, medium and long terms;
- The required skills and infrastructure for development of the solution;
- The key enablers, barriers and risks in the further development and commercialisation of the research.

At the end of the group sessions, the topics were presented to the other groups for further comments and clarifications.

TOPIC 1: PROTON EXCHANGE MEMBRANE WATER ELECTROLYSERS

1A: Decrease or Eliminate Precious Metals from Catalysts (HA3 and HA4)

This topic explored anode catalysts for PEMWEs. There are two main aspects in this domain; a) improving the performance of precious metal catalysts, specifically iridium- and ruthenium- based materials for oxygen evolution, and b) discovering non-precious metal catalysts for oxygen evolution.[37]

In order to improve the economic viability of PEMWEs for energy conversion, the system needs to be efficient and durable, and the stack components recyclable. Energy efficiency of the cell decreases with increasing current density because higher cell potentials are required at elevated current densities.[38]

A state-of-the-art PEMWEs electrolyser, operating at 1.8 A/cm^2 at 1.7 V requires 1 – 3 mg/cm^2 [39,40,41,42] of platinum group metals at the anode, typically Ir and Ru based oxides, in order to catalyse O_2 evolution. Conversely, H_2 evolution can be catalysed with negligible potential losses, or overpotentials, at ultra-low Pt loadings of 0.025 mg/cm^2. [43,44]

In the context of scaling PEMWEs to the TW scale, the reliance on such precious metals requires consideration of both availability and potential demand. For example, if one considers that the annual production of Ir and Pt are ~9 t/yr and ~200 t/yr, [45] respectively, a PEMWE electrolyser operating at 1.79 V and 3.6 A/cm^2 with 1.6 mg/cm^2 Ir and 0.025 mg/cm^2 Pt loadings, [46] a back-of-the-envelope calculation shows that >27 years and 0.02 years of entire, worldwide production produces just 1 TW of PEMWE capacity. Clearly, these calculations show that the Pt loading at the cathode *does not* pose a significant challenge to PEMWE scale-up; conversely, the Ir loading poses a much a greater bottleneck. The calculations highlight the need to develop new catalysts that utilise significantly lower Ir- without compromising catalyst activity or durability, unless other mitigation strategies become commercially viable. Beyond Ir usage, it is also important to consider the recyclability, scalability and processability of catalyst materials at scale. Such considerations will influence the overall amount of noble metal in circulation.

As a result of the limited Ir availability, a significant reduction is necessary to enable the deployment of PEMWEs at the TW scale. It is anticipated that, a reduction by a factor of ~40 Ir-loading (~0.05 mg/cm^2) is required. [47] If all these targets are achieved by the 2035 -2050 timescale, then 100% of the required hydrogen generation would be possible. It will also be important to have significant commercial interest to take that forward.

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[37] Ayers, K. *et al.* 'Perspectives on Low-Temperature Electrolysis and Potential for Renewable Hydrogen at Scale', Annual Review of Chemical and Biomolecular Engineering, 10(1), 2019 pp. 219–239. doi: 10.1146/annurev-chembioeng-060718-030241.
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[43] Bernt, M., *et al.* 'Analysis of Voltage Losses in PEM Water Electrolyzers with Low Platinum Group Metal Loadings', Journal of The Electrochemical Society, 165(5), 2018 pp. F305–F314. doi: 10.1149/2.0641805jes.
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[46] Bernt, M., *et al.* 'Analysis of Voltage Losses in PEM Water Electrolyzers with Low Platinum Group Metal Loadings', Journal of The Electrochemical Society, 165(5), 2018 pp. F305–F314. doi: 10.1149/2.0641805jes.
[47] Bernt, M. *et al.* 'Current Challenges in Catalyst Development for PEM Water Electrolyzers', Chemie-Ingenieur-Technik, 92(1–2), 2020 pp. 31–39. doi: 10.1002/cite.201900101.

Strategies[48, 49, 50] to reduce OER catalyst precious metal content have included the investigation of alloys and mixed-metal oxide phases (*e.g*. perovskites, hollandites and pyrochlores) containing both Ir (and Ru) and non-PGM metals. Other approaches, probing compositional, structural and coordination manipulations with the ultimate goal of increased iridium utilisation and packing densities, offer a broad area of research towards reducing precious metal loadings. For instance, single-atom catalysts (SACs)[51, 52,] have shown some promising activity in short-term lab-scale testing; however, there remains significant room for improvement, especially in terms of stability.

In acidic electrolyte, beyond Ir and Ru based oxides, very few materials are even moderately stable or active for the OER. Thus, the high-risk but high-reward development of completely non-precious metal OER catalysts is desirable. Indeed, recent work has highlighted a limited selection of mixed metal oxides (e.g. MnO_x-Ti,[53] and intermetallic alloys (e.g. Ni_2Ta [54,55,56]) as potential non-PGM OER candidates. However, while few such materials have shown some promising short-term lab-scale stability, the activity of the non-PGM catalysts does not rival that of Ir-based materials, at least in PEMWEs (in alkaline media non-PGM catalysts are far more stable: see Topic 2).

Overall system durability is dependent on the mode of operation (constant *vs* intermittent load), operating load and system configuration[57,58]. Typically, degradation of 3-5 µV/h are acceptable at >1A/cm^2 operating in constant load[59]. It is desirable to keep the degradation rate to the minimum, but higher degradation rates (> 20 µV/h) may have to be allowed for intermittent operations, higher current densities and low catalyst loadings. In particular, most academic studies lack rigorous tests for measuring stability; underlying corrosion processes (the dissolution of RuO_2, IrO_2 or carbon supports) are too slow to be captured by short-term electrochemical tests but significant enough to cause major degradation over the lifetime of an electrolyser, *i.e*. many years. [60] For instance, carbon-based materials are highly unstable at the potentials required to drive O_2 evolution.[35] Greater emphasis needs to be placed on understanding the degradation mechanisms and the measurement of dissolution products using ultrasensitive measurement tools; for exampleelectrochemical mass spectrometry[61] for measuring CO_2 or CO from carbon oxidation or online inductively coupled plasma mass spectrometry (ICP-MS)[62] for metal dissolution. Short-term electrochemical tests alone are insufficient.

Beyond catalyst and materials discovery, the need to develop *operando* and *in situ* characterisation methods and tools (both National Facility and lab-scale) is considered important for proving fundamental insights for catalyst design. In assessing the performance of OER catalysts, there are several figures of merit, including catalyst activity (overpotentials, intrinsic, specific, mass, and geometric, *etc*.) and durability (*i.e.* dissolution rates and stability of potential or

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current). Furthermore, the development of methods to assess catalysts integrated into catalyst layer structures (grading of layers, nanostructured thin films, radical scavengers), is important and may assist in achieving the reduction of precious metal loading. Such measurements will require standards to facilitate comparison of the data and benchmark new developments against well-characterised performance and lifetime metrics.

The limited supply of Ir presents opportunities for the development of novel materials: the development and discovery of anode catalysts that function at pH 0 with a 40-fold decrease [63,64,65] in Ir content relative to current state-of-the-art catalysts without compromising performance is a key objective. The development of high surface area stable and conducting supports and microporous transport layers would enable significantly improved Ir dispersion, over the current unsupported catalysts used in PEMWEs (see Topic 1B). [66] Material recovery, recycling and circular thinking should also be considered. Table 5 (below) shows the roadmap and the current and future performance requirements for this topic.

Table 5: Roadmap for the decrease or elimination of precious metals from catalysts topic

What is in scope	1. Fundamental research and understanding of activity and degradation mechanisms for Ir and Ru materials in PEMWE electrolyser anodes and ultralow Pt loadings in PEMWE electrolyser cathodes. 2. Development and investigation of catalyst-support interactions. 3a. Developing materials with reduced PGM content, for instance by combining PGM with non PGM materials. 3b. Designing and synthesising new materials (available and environmentally friendly), utilising knowledge gained from (points 1 and 2). 3c. Development of relevant and reliable accelerated testing protocols and benchmarking, leading ultimately to international standards. 3d. Design and characterisation of new catalyst layer structures, developing an understanding of catalysts as part of a catalyst layer, as well as in isolation. 4. Producing systems in large-scale material-processing routes and methodologies for making electrodes in large areas with high reproducibility. 5. Routes and methods for establishing and separating PEMWE-EL materials (recyclability).
What is out of scope	
Link to challenges	- Public perception and education (C1) - Hydrogen is not naturally occurring and takes huge amount of energy to release. A critical issue is where the electricity to undertake electrolysis would originate from (C2) - There is need for grid scale storage topics, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore, significant materials innovation and systems integration are required (C4) - Carbon-Neutral Aviation Fuel (C7) - Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point (C9)

	Targets				
	Efficiency %	**Scalability potential to 1 TW**	**Durability**	**Recyclability (end of life)**	**Carbon Footprint $kgCO_2e/MWh$ (cradle-to-grave)**
Anticipated impacts this topic may have on the targets by 2050	>80% LHV, at 2-5 A/cm^2 and 30 bar H_2 output and 50 ° C.	Resource availability of the material needs to be considered (an overarching principle)/utilisation of low-toxicity, environmentally friendly materials.	40,000-100,000 h operational lifetime and ability through several thousands of shut down cycles; degradations of 3-5 µV/h at >1A/cm^2 constant load[67].	PGM: easy to recycle and can be fed into the front end of the system; research questions around non-PGM (from other components of electrolyser) and cost-effectiveness	Wind electrolysis: 9.4 -21.4 g CO_2e/kWh, solar PV electrolysis: 25 – 48 g CO_2e/kWh, nuclear electrolysis: 8.4 – 18 g CO_2e/kWh [68]; needs better understanding.

63 Bernt, M. *et al*. 'Current Challenges in Catalyst Development for PEM Water Electrolyzers', Chemie-Ingenieur-Technik, 92(1–2), 2020. pp. 31–39. doi: 10.1002/cite.201900101.
64 Ayers, K. *et al.* 'Perspectives on Low-Temperature Electrolysis and Potential for Renewable Hydrogen at Scale', Annual Review of Chemical and Biomolecular Engineering, 10(1), 2019, pp. 219–239. doi: 10.1146/annurev-chembioeng-060718-030241.
65 Carmo, M. *et al*. 'A comprehensive review on PEM water electrolysis', International Journal of Hydrogen Energy, 38(12), 2013 pp. 4901–4934. doi: 10.1016/j.ijhydene.2013.01.151.
66 Bernt, M., *et al.* 'Analysis of Voltage Losses in PEM Water Electrolyzers with Low Platinum Group Metal Loadings', Journal of The Electrochemical Society, 165(5), 2018 pp. F305–F314. doi: 10.1149/2.0641805jes.
67 Ayers, K. E., *et al.*, 'Fueling Vehicles with Sun and Water', ECS Transactions 50, no. 49, 2013, https://doi.org/10.1149/05049.0035ecst.
68 Parkinson, B., *et al.* 'Levelized cost of CO 2 mitigation from hydrogen production routes', Energy and Environmental Science. Royal Society of Chemistry, 12(1), 2019, pp. 19–40. doi: 10.1039/c8ee02079e.

<table>
<tr><td rowspan="2">Current and future performance</td><td colspan="2">Current state-of-the-art</td><td>Desired future. Key performance characteristics / parameters</td></tr>
<tr><td colspan="2">Metal-oxides supported Ir and Ru based catalysts;
1-3 mg/cm^2 loading;
1.7 – 1.8 V and 3.6 A/cm^2 [69];
There are many examples of durability studies.
One recent example of state-of-the-art: square wave AST protocol (3 A/cm^2, 10 mins, 0.1 A/cm^2 10 mins) – no degradation observed over 500 cycles [70, 71]. However, it is unclear how well the performance in accelerated degradation tests corresponds to long-term degradation tests.</td><td>Highly efficient catalysts, with long lifetimes (see targets)</td></tr>
<tr><td></td><td>Short-Term
2020 - 2025</td><td>Medium-Term
2025 – 2035</td><td>Long-Term
2035 - 2050</td></tr>
<tr><td>Technology Research and development path towards the desired future. Key milestones.</td><td>-Identify mechanisms for activity and degradation;
-Develop accelerating testing protocol;[72] for non-PGM: catalysts experimental and computational screening for potential candidate materials.</td><td>-Identify promising non-PGM catalysts with PGM like performance 1 A/cm^2 at 1.7 Volts (but recognising this is unlikely to have long-operational lifetime);
-Large scale materials processing optimisation for reduced precious metal catalysts.</td><td>- 40-fold reduction in Ir (or Ru) loading (~0.05 mg/cm^2) without compromising performance or durability at 4-5 A/cm^2 and 1.7 V.
high performance and long lifetime for non-PGM materials.</td></tr>
<tr><td>Required competences and resources (finance, people, knowledge, partnerships etc.)</td><td colspan="3">• Funding opportunities to support the development of the described research (above), supporting studentships and, postdoctoral researchers, to train the next generation of scientists, providing support for both academic research, and industrial-academic collaboration; CDT centres that bridge the gap between industrial scale and lab-scale catalysts
• UK workforce that is knowledgeable in the field of catalysis for H_2 production (follows on from CDT centres captured in ST).
• Academic, research institute, and industrial collaboration.
• Training and education of researchers (in the UK there is a lack of critical mass of researchers working in this space); computational chemists; CDT centres that focus on for example, industrial scale rather than lab-scale catalysts.
• Develop a broad range of characterisation techniques to be able to measure operando performance and understand reaction mechanisms and degradation pathways for example table-top synchrotron capabilities within the UK for characterising catalysts in-operando.
• UK workforce that is knowledgeable in the field of catalysis for H_2 production (follows on from CDT centres captured in ST).</td></tr>
<tr><td>Expected deployment (%) (linked to 1TW installed capacity)</td><td><1%</td><td><10%</td><td>Approaching 100% (if the targets are met)</td></tr>
<tr><td>Technology enablers</td><td colspan="3">• Professional, independent facilities for short and long-term operando testing (including synchrotron facilities and neutron imaging) and validation of new materials under the relevant conditions. Imaging of catalyst layers in-situ and ex-situ testing.
• Facilities for rigorous stability measurements, going beyond short-term electrochemical measurements, e.g. inductively coupled plasma mass spectrometry
• Operando, in situ, and ex situ atomic resolution characterisation of catalysts and catalyst-support interactions to elucidate catalytically active surface and interface structures and their dynamic evolution at critical length scales.
• National electron microscopy facilities (e.g. SuperSTEM, the EPSRC National Research Facility for Advanced Electron Microscopy) for atomic resolution imaging and spectroscopy of single atom catalysts, catalyst and support surfaces and interfaces including at process conditions, e.g. variable temperature/in situ microscopy.
• High throughput testing for new and novel catalyst motifs; including engaging with computational chemists.
• Partnerships: an interaction between academic and industrial partners who understand how things will operate in a stack and what the real need is, academics who can develop new</td></tr>
</table>

[69] Bernt, M., *et al.* 'Analysis of Voltage Losses in PEM Water Electrolyzers with Low Platinum Group Metal Loadings', Journal of The Electrochemical Society, 165(5), 2018, pp. F305–F314. doi: 10.1149/2.0641805jes.
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	materials and methods and research institutes who can bridge the gap and support scale-up and testing. For example, in participation in Horizon Europe. • Facilities for *in-operando* testing of catalysts. • High throughput testing for catalysts. • Imaging of catalyst layers *in-situ* and *ex-situ* testing (already done in fuel cells). • Access to synchrotron facilities and neutron imaging. • Table-top synchrotrons (groups in Korea and China working on these). • Resources: capital. • Moving toward single-atom catalysts to reduce the amount of Iridium catalysts used, using matrices or supports that will be stable for the 40,000 to 100,000 hours lifetime required of an electrolyser. • Simulation tools to discover new materials *in silico*. This is key to accelerating material discovery (R1). • Analytical techniques for driving real understanding of the conversion processes and allows us to "see" what's going on in real time. Generating understanding of processes for optimisation (R2). • Identification of active catalyst state (R3). • Fundamental surface science of for example electrolysis, catalysis, steam reforming, etc. the processes that make hydrogen (R8). • Better understanding of reaction mechanisms (R11). • Reduced or even non-precious metal content catalyst layers for PEMWE (R13).
Commercial enablers	• Ability and desire to scale up to TW level. • Market pull for hydrogen; cheap access to renewable electricity. • Capability to manufacture the systems on a large-scale. • Policy and political will (net -zero targets). • Curricular systems to fill the skills gap. • A mechanism for translating promising low-PGM content catalysts from the lab-scale to commercial-scale, providing opportunities that recognise the disparate expectations between academic and industrial manufacturers. A mechanism for scaling up catalysts that can be commercially tested would be very helpful, for example by having industry-university links through Innovate-type programmes or University strategic fund programmes that help to scale up materials. • Fully funded government programmes that support joint industry-research partner projects that will output over the medium (5-10 year) term., with a program structure similar to the EU's Fuel Cell and Hydrogen Joint Undertaking (FCHJU) projects. • ARPA-type programmes for the UK in catalysis or energy in general.

1B: Develop New Conductive and Stable Materials for PEMWE Current Collectors, Porous Transport Layers and Catalyst Support

This topic discussed materials development for the PEMWE structural components including catalyst supports, porous transport layers, current collectors, bipolar plates and end plates. The overall system development was also considered, as the material choices will affect the system design and operation.

Structural component degradation also increases cell potentials due to increased interfacial contact resistance and poor mass transport. With the exception of membrane, transport layers and gaskets, most metallic PEMWE stack components can be recycled/reused with appropriate processing, modifications and machining. Catalysts are recovered by leaching, precipitation and purification.[73] Current collectors, bipolar plates and end plates can also be reused by reprocessing and replating the protective layers. [74] However, as with the cost for the beginning of life (BOL) materials processing and manufacturing, the cost of recovering and processing at the end of life (EOL) is currently the primary barrier. [75]

[73] Valente, A., *et al.*, 'End of life of fuel cells and hydrogen products: From technologies to strategies', International Journal of Hydrogen Energy 44, no. 38 2019, https://doi.org/10.1016/j.ijhydene.2019.01.110.
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[75] Mayyas, A.T, *et al.*, 'Manufacturing Cost Analysis for Proton Exchange Membrane Water Electrolyzers', United States: N. p., 2019. Web. doi:10.2172/1557965.

Catalyst Support

Employing supports for PEMWE anode catalysts akin to Pt/C in PEMWE fuel cells will improve precious metal catalyst usage (see Topic 1a). However, carbon and earth abundant metals cannot be used since they will readily oxidise. Oxides like TiO_2 are stable under the PEMWE anode operating environments but they are poor conductors. To compensate for the extremely low TiO_2 conductivity, the commercial IrO_2-TiO_2 catalysts consists of 75 wt% IrO_2[76]. Additionally, TiO_2 supported IrO_2 catalyst processing cost is high since they do not benefit from economy of scale. Currently, the unsupported Ir catalysts are economically more viable, and thus, considered state-of-the-art rather than the 75 wt% IrO_2-TiO_2. Another area of active investigation is to improve conductivities of metal oxide by doping or preparing oxides with oxygen vacancies. Conductivities of doped and sub-stoichiometric oxides are orders of magnitude higher than conductivities of metal oxides, but the dopants tend to leach out and the stoichiometry revert to insulating phases under the highly oxidising PEMWE electrolysis conditions[77]. Development of a conductive, economic and electrochemically stable catalyst support is thus a research priority for PEMWEs[78,79].

Transport and Structural Layers

Similar to catalyst supports, other PEMWE components also need to be highly conductive and resistant to oxidation. The need to use high -quality Ti and the expensive manufacturing process for Ti transport and structural layers constitutes a major portion (64%) of the total stack capital cost.[8] Recent advancements in manufacturing processes and re-engineering various components have reduced the cost emanating from flow fields and bipolar plates by 55%. Similar system and component rethinking needs to be carried out throughout the process, namely, component design to system configuration. Additionally, titanium oxidises and passivates rapidly under the anodic oxygen evolution reaction (OER) conditions. The only viable option currently available to protect titanium transport components, such as porous transport layers (PTLs), flow fields, bipolar plates and end plates, is to coat the surface with a thin layer of platinum group metals (PGMs). [80,81] A conformal layer of Pt or Ir reduces interfacial resistance and also improves the durability of PEMWEs.[82] However, additional capital costs of depositing 0.1-0.2 mg/cm^2 (100-200 nm) PGM over the titanium surfaces are significant. [83] More economic substitutes for protective layer coatings, materials beyond titanium and titanium processing need to be investigated. [84] Microporous layers (MPLs) in fuel cell membrane electrode assemblies (MEAs) regulate mass transport as well as maintain robust interfacial contact between the catalyst layer and gas diffusion layers (GDLs). [85] Analogous MPLs for PEMWE anode PTLs have not been developed, but recent reports have shown improved performance upon changing PTL porosity and adding a MPL layer. [86] This area of optimising component architectures such as PTL porosity and MPL and manufacturing processes should be prioritised as a research area; taking inspiration from fuel cell and battery technologies.

[76] Ayers, K., *et al.,* 'Perspectives on Low-Temperature Electrolysis and Potential for Renewable Hydrogen at Scale' Annu Rev Chem Biomol Eng, 10, 2019. https://doi.org/10.1146/annurev-chembioeng-060718-030241.
[77] Han, B., *et al.,* 'Screening Oxide Support Materials for OER Catalysts in Acid', Journal of The Electrochemical Society 165, no. 10 2018, https://doi.org/10.1149/2.0921810jes.
[78] Bernt, M., *et al.,* 'Current Challenges in Catalyst Development for PEM Water Electrolyzers', Chemie Ingenieur Technik 92, no. 1-2 2019, https://doi.org/10.1002/cite.201900101.
[79] Zhang J., *et al.,* 'Support and Interface Effects in Water-Splitting Electrocatalysts', Adv Mater 31, no. 31 2019. https://doi.org/10.1002/adma.201808167.
[80] Liu, C., *et al.,* 'Performance enhancement of PEM electrolyzers through iridium-coated titanium porous transport layers', Electrochemistry Communications, 97, 2018, https://doi.org/10.1016/j.elecom.2018.10.021.
[81] Jung, H-Y., *et al.,* 'Performance of gold-coated titanium bipolar plates in unitized regenerative fuel cell operation', Journal of Power Sources 194, no. 2, 2009, https://doi.org/10.1016/j.jpowsour.2009.06.030.
[82] Jung, H-Y., *et al.,* 'High-durability titanium bipolar plate modified by electrochemical deposition of platinum for unitized regenerative fuel cell (URFC)', Journal of Power Sources 195, no. 7, 2010, https://doi.org/10.1016/j.jpowsour.2009.10.002.
[83] Christoph R. *et al.,* 'The stability challenge on the pathway to high-current-density polymer electrolyte membrane water electrolyzers', Electrochimica Acta 278 2018, https://doi.org/10.1016/j.electacta.2018.04.154.
[84] Yang, G., *et al.* 'Bipolar plate development with additive manufacturing and protective coating for durable and high-efficiency hydrogen production', Journal of Power Sources, Volume 396, 2018, Pages 590-598, https://doi.org/10.1016/j.jpowsour.2018.06.078 .
[85] Weber, A.Z., and Newman, J., 'Effects of Microporous Layers in Polymer Electrolyte Fuel Cells', Journal of The Electrochemical Society 152, no. 4, 2005, https://doi.org/10.1149/1.1861194.
[86] Schuler, T,. *et al.,* 'Hierarchically Structured Porous Transport Layers for Polymer Electrolyte Water Electrolysis', Advanced Energy Materials 10, no. 2, 2019, https://doi.org/10.1002/aenm.201903216.

Degradation Mechanisms

Degradation mechanisms of PEMWE transport and structural components are essential to the development of more efficient, cost- effective and durable materials. Most of the electrolyser components, their geometry and assembly are directly borrowed with some subsequent modifications from fuel cells. [8] Although seemingly very similar in assembly and operation, PEMWEs also differ fundamentally from PEMWE fuel cells. For example, electrolyser membranes are much thicker (<25 microns vs around 175 microns), the cell needs to be flooded in liquid fed mode, as such pressures are unbalanced and a magnitude higher (3.5 bar in fuel cell vs 30 bar in electrolyser) resulting in different thermal management needs due to the underlying overall chemical reaction (exothermic in fuel cell but endothermic in electrolyser).[8,10,87] Optimising each component for electrolyser specific applications and deconvoluting degradation pathways will be essential for further performance and durability improvements. Among other things, such efforts can benefit from standardised protocols for each component as well as for overall cell/stack performance specific for end application. The United States Department of Energy[88] and the European Union Joint Research Centre[89] have formulated targets and guidelines for hydrogen production, but PEMWE specific consortiums, preferably based on international cooperation, may be necessary – similar to the Fuel Cell Consortium for Performance and Durability (FCPAD) in the United States for fuel cells. [90]

Table 6 (below) shows the roadmap and the current and future performance requirements for this topic.

Table 6: Roadmap for the development of new conductive and stable materials for PEMWE current collectors, porous transport layers and catalyst support topic

What is in scope	• Transport and structural layers: materials, coatings and morphology • Device and component durability • Interactions between membranes, catalysts and catalyst supports • Materials choices • MEA membrane additives				
What is out of scope	• System design • System costs				
Link to challenges	• Integrated energy network (C2) • Grid scale energy storage (C4) • Industrial sector - reforming, ammonia, minerals, etc. (C6) • Viable technologies (C8) • Decarbonisation of industrial processes (C9) • Hydrogen delivery network (C12)				
	Targets (to be achieved by 2050): aligned with other PEMWE targets				
	Efficiency %	**Scalability potential to 1 TW**	**Durability**	**Recyclability (end of life)**	**Carbon Footprint $kgCO_2e/MWh$ (cradle-to-grave)**
Anticipated impacts this topic may have to the targets by 2050	See Figure 10	-Component recyclability. -Materials processing costs. -See Figure 10	-See Figure 10	- Membrane, GDLs , and gaskets not recyclable. - Metal components are recyclable,	--See Figure 10

[87] Babic, U., *et al.*, 'Understanding the effects of material properties and operating conditions on component aging in polymer electrolyte water electrolyzers', Journal of Power Sources 451, 2020, https://doi.org/10.1016/j.jpowsour.2020.227778.
[88] US Department of Energy: The Hydrogen and Fuel Cell Technologies Office 'Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan', 2015 https://www.energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf.
[89] Bertuccioli, L., *et al.*, 'Study on development of water electrolysis in the EU' Comissioned by Fuel Cells and Hydrogen Joint Undertaking https://www.fch.europa.eu/sites/default/files/FCHJUElectrolysisStudy_FullReport%20(ID%20199214)
[90] Fuel Cell Performance and Durability, https://www.fcpad.org/ .

<table>
<tr><td></td><td></td><td></td><td></td><td>and many are reusable.
- Recyclability expected to improve as the industry matures.
- Cost is critical for reactivation and reuse.</td><td></td></tr>
<tr><td rowspan="2">Current and future performance</td><td colspan="3">Current state of art[8,10]</td><td colspan="2">Desired future</td></tr>
<tr><td colspan="3">• PTL, BPP, endplates, support mesh – Ti, 0.1-0.2 mg/cm² PGM</td><td colspan="2">• PTL, BPP, endplates, support mesh – low grade Ti, steel, PGM free and low processing costs</td></tr>
<tr><td></td><td colspan="2">Short-Term
2020-2025</td><td colspan="2">Medium-Term
2025-2035</td><td>Long-Term
2035-2050</td></tr>
<tr><td>Technology research and development path towards the desired future. Key milestones.</td><td colspan="2">• Consensus in performance parameters
• Diagnostic techniques to understand device and component failure mechanisms at microscopic scale
• Efficient and durable materials combining theory and experiment
• Control PTL porosity without losing conductivity
• Low hydrogen cross over MEAs at high differential pressure.</td><td colspan="2">• Electrolyser specific cell/stack configurations and components.
• Titanium replacement (cheaper alloys or more economic elements).
• Develop MPL for the anode PTL.
• Efficient and economic water purification technology at elevated temperatures (> 60 °C).
• Cost-effective materials processing and recycling technologies.
• Conductive and stable oxide catalyst supports.
• Device and materials modelling for materials discovery and system improvements.
• Holistic research approach with synergy among chemistry, physics, materials science and other disciplines.</td><td>• Make the system more tolerant to load fluctuations and impurities.
• Vapour feed electrolysis for water deficient environments.
• Self-healing materials</td></tr>
<tr><td>Required competencies and resources (finance, people, knowledge, partnerships etc.)</td><td colspan="5">• Clear technology transfer routes from academic labs to industry.
• Standardise PEMWE test protocols targeted for end applications.
• Separate standards and protocols for academia and industry.
• Material specific guidelines for academic labs and industry.
• Develop operando characterisation techniques for atomic, macroscopic and device level diagnosis.
• Interdisciplinary approach is needed: electrochemists, metallurgists, material scientists and modelling.
• Academic institutions train graduates and postgraduates to prepare for scaled up renewable energy industry.</td></tr>
<tr><td>Expected deployment (%) (linked to 1TW installed capacity)</td><td colspan="2"><1%</td><td colspan="2"><10%</td><td>approaching 100% (if the targets are met)[91]</td></tr>
<tr><td>Technology enablers</td><td colspan="5">• Accelerated materials discovery via theory driven investigations. (R1)
• In operando/in situ investigations to establish materials degradation and system failure. (R2)
• Improved surface science and engineering techniques and fabrication methods to understand catalysis and interfacial phenomena (R8)
• Establish reaction/degradation mechanisms (R11)
• Scaled up and economic renewable, for example wind power, hydroelectric, solar etc. (R15)</td></tr>
<tr><td>Commercial enablers</td><td colspan="5">• Increased synergy between academic research and industry
• Identify niche market that can readily integrate hydrogen, oxygen and fuel cells at scale.
• Economic and policy support from governments (local, regional and national).</td></tr>
</table>

[91] Dodds, P.E., *et al.,* 'Opportunities for hydrogen and fuel cell technologies to contribute to clean growth in the UK' H2FC Supergen, University College London, UK, 2020, http://www.h2fcsupergen.com/opportunities-for-hydrogen-fuel-cell-tech-growth-uk .

	• Legislative regulations to persuade industries such as, green hydrogen use in refineries. • Business cases that highlight the benefits of green hydrogen rather than blue and grey hydrogen. • Work initially at small but highly visible cases to influence public perception. • Highlight the benefits of distributed generation. • 2030 problem: renewable electricity generation will outpace existing grid capacity; hydrogen is a technology ready solution to fill the gap.

TOPIC 2: WATER ELECTROLYSIS IN ALKALINE MEDIA: IMPROVE MEMBRANE STABILITY AND CONDUCTIVITY AND CATALYST ACTIVITY

This topic explored materials for electrolysers operating in alkaline electrolysers. These devices have fundamentally different materials requirements to those operating in acid which potentially offers significant CAPEX savings compared to state -of the -art PEMWE technology due to lower membrane and electrode costs. The principal advantages of operating in alkaline conditions are the relative stability of transition metals and their oxides. This allows alkaline electrolysers to operate without the use of critical raw materials (CRM) such as iridium. The fundamental challenges are (i) the slower kinetics of hydrogen evolution in alkaline conditions; and (ii) the lower conductivity and stability of hydroxide-conducting polymeric electrolytes, relative to proton conducting counterparts. The two types of alkaline electrolysers, AWE and AEMWEs share *some* materials challenges, so both are within the scope of this topic.

AWE and AEMWE provide the opportunity for very low CAPEX electrolysers (which may produce hydrogen from renewables at a lower cost and with smaller CO_2 footprint than reforming technologies. The UK currently has little research activity in alkaline systems (aqueous and solid polymer) and there is limited commercial interest, which could change in the medium-term. A British industrial champion could be very influential in driving further developments in this area for the UK.

Table 7 (below) shows the roadmap and the current and future performance requirements for this topic.

Table 7: Roadmap for water electrolysis in alkaline media: improve membrane stability and conductivity and catalyst activity topic

What is in scope	• Both alkaline water electrolysers (AWE) and anion exchange membrane water electrolysers (AEMWE). • All materials, including (but not limited to): catalysts, membranes, separators, transport layers, current collectors, ionomers, binders, MEA additives, balance of plant components, radical scavengers and membrane reinforcements. • Both materials and components – for instance, the structure of a catalyst layer, not just the alloy composition chosen. • Interfaces between materials – for example, specific absorption of cations onto catalysts. • Holistic approaches that consider that materials and components must work at real operating conditions present in full-scale, deployed systems. • Both performance and durability. • Hydrogen evolution and oxygen evolution reactions in alkaline media. • Processes to produce components, for example, novel methods of processing catalyst layers or membranes. • Materials challenges that relate to scalability, recyclability, second-use production, for example, scalable catalyst/membrane production and quality control. • Development of new testing techniques and facilities. • Better tools for finding new materials, computational and high throughput screening.
What is out of scope	• Non-material issues, except where they relate to understanding materials. For instance, system modelling to understand temperature range materials must be stable, so is in, while system modelling to optimise systems is out.
Link to challenges	• Public perception and education (C1). • Hydrogen is not naturally occurring and takes a huge amount of energy to release. A critical issue is where the electricity to undertake electrolysis would originate from (C2). • Hydrogen is difficult to store and distribute (C3). • There is a need for grid-scale storage solutions, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore, significant materials innovation and systems integration are required (C4).

<table>
<tr><td></td><td colspan="5">• The main production technologies that produced reasonable volumes of compressed hydrogen are not practically scalable, and thus it is essential that alternatives are found (C5).
• Viable technologies (C8).
• Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point (C9).
• Subsidies to ensure competitiveness (C11).
• UK-wide H_2 delivery network at appropriate H_2 purity for maximum impact (C12).
• Policy and regulation for hydrogen economy (C13).</td></tr>
<tr><td rowspan="3">Anticipated impacts this topic may have to the targets by 2050</td><td colspan="5">Targets</td></tr>
<tr><td>Efficiency %</td><td>Scalability potential to 1 TW</td><td>Durability</td><td>Recyclability (end of life)</td><td>Carbon Footprint $kgCO_2e/MWh$ (cradle-to-grave)</td></tr>
<tr><td>AEMWE:
>80% LHV, at 2-5 A/cm^2 and 30 bar H_2 output, i.e. equal to PEMWE electrolysis (see Topic 1)

AWE:
80% @ 1 A/cm^2 at 10 bar H_2 output.</td><td>No critical raw materials (Pt/IrO_x) are required and production processes exist or can be adapted from PEMWE. Business case for investment in factories to produce at scale is challenging.

AEMWE:
No fundamental issues

AWE:
Historically deployed at 100 MW</td><td>AWE have already demonstrated decades of stability. For AEMWE durability is a key research challenge.

AEMWE:
40,000-100,000 h operational lifetime and through several thousands of shut down cycles; degradations of 3-5 µV/h at >1A/cm^2 constant load[92].

AWE:
100 000 h, <10% loss @ nominal current.</td><td>AEW & AEMWE:
Recyclability, second life and reusability should be similar to other electrolyser technologies and are not seen to be an issue. Full lifecycle assessments would be required especially around mining of materials and toxicity etc. but nothing intrinsically difficult.</td><td>AWE & AEMWE:
Strongly depends on source electricity. Should be similar to other technologies but needs better studies.

CCC estimates indirect emissions from electrolysis by 2050 to be 11-14 gCO_2/kWh, assuming a decarbonised energy grid. Compared to reforming lifecycle emission[93] of 29-120 g CO_2e/kWh even with CCUS.

Wind electrolysis: 9.4-21.4 g CO_2e/kWh, solar PV electrolysis: 25 – 48 g CO_2e/kWh, nuclear electrolysis: 8.4 – 18 g CO_2e/kWh[94];</td></tr>
<tr><td rowspan="2">Current and future performance</td><td colspan="3">Current state-of-the-art</td><td colspan="2">Desired future. Key performance characteristics / parameters</td></tr>
<tr><td colspan="3">AEMWE:
Prototype systems <5 kW are under development or available from start-ups. EU call[95] at TRL3/4 requires a 1 kW stack with a minimum of 5 cells reaching single-cell voltages of 2 V at 1 A cm^{-2} at 45°C and to maintain stable performance at constant current for 2,000 h with a degradation gap of less than 50 mV.

Prototype AEM are under development by various companies/ universities: Evonik, Ionomer etc. AEM specific KPI's were area specific resistance ≤ 0.07 Ω cm2 (room temperature), a swelling ratio (dry/wet) ≤ 1 % in machine direction and ≤ 4 % in transverse direction,</td><td colspan="2">Main key performance indicator for all electrolysers is the ability to produce levelised cost of H_2 lower than SMR/ATR ca. £27-46/MWh[97].

AEMWE:
Performance comparable to PEMWE but with no/low PGM use at anode or cathode. Ability to follow loads and operate with differential pressure.

AWE:
CAPEX costs < 200 USD kW^{-1} with efficiency of 80%.</td></tr>
</table>

[92] Ayers K.E., *et al.*, 'Fueling Vehicles with Sun and Water' ECS Transactions 50, no. 49 2013, https://doi.org/10.1149/05049.0035ecst.
[93] Committee on Climate Change, 'Hydrogen in a low-carbon economy' 2018, https://www.theccc.org.uk/wp-content/uploads/2018/11/Hydrogen-in-a-low-carbon-economy.pdf
[94] Parkinson, B. *et al.* 'Levelized cost of CO_2 mitigation from hydrogen production routes', Energy and Environmental Science. Royal Society of Chemistry, 12(1), 2019 pp. 19–40. doi: 10.1039/c8ee02079e.
[95] Fuel Cell and Hydrogen Joint Undertaking, Funding Call H2020-JTI-FCH-2019-1, https://www.fch.europa.eu/page/call-2020
[97] Committee on Climate Change, 'Hydrogen in a low-carbon economy' 2018, https://www.theccc.org.uk/wp-content/uploads/2018/11/Hydrogen-in-a-low-carbon-economy.pdf

	mechanical strength of 15 MPa, elongation at break of 100 %, conductivity: 20 mS cm^{-1}. **AWE:** Well-developed commercial stacks ~2.5 MW are already available on the market[96]. 100 MW installations are known. The EU's MAWP 2020 targets/status are 49 kWh kg^{-1} at 0.7 A cm^{-2}, 600 Euro kW^{-1} and degradation of 0.12% per 1000h.		
	Short-Term **2020 - 2025**	**Medium-Term** **2025 - 2035**	**Long-Term** **2035 - 2050**
Technology Research and development path towards the desired future. Key milestones.	**AEMWE:** Membranes with better long-term stability, temperature stability, material robustness both mechanically and dimensionally (swelling). Developing existing approaches such as cross-linking of polymers or building on those approaches used for PEMWE such as developing composites with thin reinforcement layers and radical scavengers etc. Development of non-PGM catalysts with equivalent PEMWE performance and incorporation into high performance catalyst layers/ MEA. In particular, improved non-PGM hydrogen evolution catalysts will be crucial. The activity of platinum is reduced ~100 fold in alkaline electrolytes[98] relative to the acid electrolytes used in PEMWEs. There are even high potential losses for non-precious metal catalysts in alkaline media. New and improved hydrogen evolution catalysts will be required in order for AEM electrolysers to compete with PEMWEs. **AWE:** Development of new separator material with same or reduced crossover and lower area specific resistance. Development of catalyst materials and catalyst layer morphologies with much higher current densities and 50% efficiency. Materials development to enable higher temperature operation. **Both:** Better *in situ / in operando* testing. Need techniques to predict performance of materials in real systems especially durability. Need new methods to understand and quantify slow degradation mechanisms. Fundamental science needed to understand the difference between hydrogen evolution in acid and alkali environments. Begin methods for developing new catalysts, for example, artificial intelligence and machine learning to identify potential new catalysts and high throughput screening technologies.	**AEMWE:** Optimisation of materials scale up to larger scale more professional materials. Systems using water circulant or weak alkali (e.g. carbonate) solutions rather than 1 M alkaline. Underlying proposition is to drive down system cost and maintain durability. Systems operating with pressure differential (20 -30 bar) **Both:** Better techniques for rapidly assessing material lifetime under different operating conditions and different end use profiles (for example, load following). Full and accurate multi-physical simulation of systems possible.	**AEMWE:** Improving materials processability, quality and lifetime for production of full commercial systems. Incremental gains in KPIs – a focus on reducing costs and increasing performance. **AWE:** Optimised materials for lowest possible CAPEX and highest efficiency. **Both:** *Ab initio* catalyst / material discovery and testing.

[96] https://nelhydrogen.com/water-electrolysers-hydrogen-generators
[98] Durst, J., *et. al.*, 'New insights into the electrochemical hydrogen oxidation and evolution reaction mechanism' Energy Environ. Sci., 7, 2255, 2014, https://doi.org/10.1039/C4EE00440J .

Required competencies and resources (finance, people, knowledge, partnerships etc.)	All these developments will require multidisciplinary skillsets from academia such as temperature measurements, polymer science, electromagnetics, etc. Currently, there are very few research groups (<5) in the UK developing membranes for electrochemical devices and no significant membrane industry. Forming a membrane centre to develop membranes will be a big enabler. Fundamental research on polymers as well as production at scale are crucial for these technologies. Enhanced testing facilities, in particular ability of research institutes to test new materials in conditions relevant for end devices. Better in situ measurements to understand degradation processes, for example a reference electrode to understand what happens in situ at the cathode and anode. Better analytical techniques for online measurements. Stronger links between industry, research institutes and academia to provide a pathway for impact for research and more communication from industry on what the challenges are. Modelling and simulation at device level for transport problems. New materials discovery techniques, for example, computational approaches and high throughput. Molecular simulation to understand the conformation of polymers, and ion transport at the molecular level. Understand where the competition is and build collaborations in the US, Asia, and Europe. A large part of the value chain for these technologies will sit outside Europe.	Better predictive tools, *operando* measurements and computational tools to carry out materials screening with a focus on predicting long-term durability/ behaviour. Strong focus for membrane producers to make membranes that are more mechanically and dimensionally, robust with high conductivity and a low swelling using scalable techniques. Roll-to-roll continuous casting process for large-scale manufacturing of membranes.	
Expected deployment (%) (linked to 1TW installed capacity)	**AWE:** 80% of electrolyser market. Older models with high CAPEX predominate. By 2025 new materials will take 25% market share of the AEM market. **AEMWE:** Available commercially at 10-100 kW scale for niche markets. <1%, mostly prototype or demonstrator devices.	**AWE:** Smaller share of electrolyser market, share shrinks as large-scale PEMWE become cheaper. Very low CAPEX ensures that it is used in markets where renewable electricity is cheap. 100% roll -out of next-generation materials for example Ni alloy catalysts and thinner separators. **AEMWE:** Available commercially in MW sized demonstration stacks and commercial scale smaller stacks. Materials are a 'drop in' replacement for PEMWE/AEM systems so scaling is easier.	**AEW:** Shrinking market share as PEMWE and AEMWE improve. Very low CAPEX means technology will still be deployed where cheaper but more intermittent renewables can be assessed. **AEMWE:** Full sized (10's MW - GW) installations commercially. Performance and durability depending it will take market share from PEMWE and AEM systems.
Technology enablers	• Simulation tools to discover new materials *in silico*. This is key to accelerating material discovery (R1). • Analytical techniques for driving real understanding of the conversion processes, which allows us to "see" what's going on in real time. Generating understanding of processes for optimisation (R2).		

	• Identification of active catalyst state (R3). • Fundamental surface science of for example electrolysis, catalysis, steam reforming, etc. the processes that make hydrogen (R8). • Better understanding of reaction mechanisms (R11)- (better understanding of reactions that cause destabilisation of the catalyst). • Reduced or even non-precious metal content catalyst layers for PEMWE (R13). • Durable, robust and active AEM membrane development (R14).
Commercial enablers	Collaboration opportunities between academia and industry are crucial. There is not sufficient co-ordination between academic research and industry activity with access for academia to testing facilities that are operated in an industrially relevant way at the full range of relevant conditions. There also needs to be an extra focus on polymer/ membrane scale-up, as there is a real challenge in commercialising these membranes. Manufacturing and scale up of materials are difficult, and support is needed. There are only a few companies carrying out alkaline electrolyser research in the UK and possibly none working on alkaline membrane electrolysers. Having a strong British champion to drive these technologies will be crucial. Funding at adequate levels is also important. This year, the EU framework funded, three €2 million projects on anion exchange electrolysers. Access to venture capital and investment is crucial for industry. The competition is substantial from both EU, USA and China. International collaboration is key. UK will not necessarily capture the entire value chain, but it could contribute significantly in producing membranes other components and exporting internationally. Numerous multi-nationals with footprint in the UK use or build AWE equipment but have limited R&D in the UK. Regulation will be critical in supporting the adoption of this technology, the cost vs SMR without CCUS is too high. Also, there is a need to understand the roles of blue and green hydrogen. Development and deployment will be limited by amount of hydrogen utilisation and infrastructures, technologies and applications (trucks, heating) Renewable energies for 100% green hydrogen: regulatory, political and/or tax incentives, for example, carbon tax and wide roll out of RES. The commercial potential of this technology is large because it has low CAPEX, so it can still be profitable in areas where renewables are very intermittent. The technology is also modular and can be deployed on a small, medium and large scale and offers the flexibility of being able to be used in both a decentralised and a centralised manner. Other drivers are the UK's high off-shore RES resources that drives hydrogen integration as well as the UK's manufacturing capability.

TOPIC 3: HIGH-TEMPERATURE ELECTROLYSIS: IMPROVE ELECTRODE AND ELECTROLYTE MATERIALS

High-temperature electrolysis can achieve very high efficiencies that are close to 100%. The high efficiency exhibited by this technology makes it an ideal candidate for industrial applications for making valuable chemicals. In addition, high-temperature electrolysis is an endothermic process requiring heat, so this technology is ideal for integration with other thermal, industrial processes. This technology integrates nicely with CO_2 capture schemes and potentially also co-electrolysis processes.

The key challenges with this technology are scalability and durability both in terms of lifetime and of dynamic response time to loading. Regarding scalability, there are two important parameters to consider: the optimum size of the high-temperature electrolyser (kilowatt, megawatt or gigawatt) and the installed manufacturing and supply chain capability. Currently, both parameters are under development and efforts are focused on understanding whether the existing technology is capable of meeting these requirements.

The materials properties are a critical factor for enabling manufacturing of electrolysis devices, both economically and at scale. If the existing materials currently used for high-temperature solid oxide electrolyser cells HRcannot be used in electrolysis mode, the technology development will take longer as an entirely new set of materials will be required. The specific hydrogen application is important too. For example, the material requirements for high-volume, high-scale, low-value applications for example, high-value chemical feedstock synthesis would be different to smaller-volume and smaller-scale opportunities such as energy storage. The operation of the system either in pure electrolysis or in a reversible mode will also affect material choices and their durability requirements. Requirements for producing hydrogen at pressure will impact cell and stack designs, and in turn materials choices,

The materials that are used currently were originally designed to operate as a solid oxide fuel cell (SOFC), so they are optimised in terms of the oxygen reduction reaction. In an electrolyser, the process is water incorporation and then migration of either oxide ions into an oxide ion conducting electrolyte, and the release of hydrogen or in a proton conducting electrolyte, the migration of protons into the electrolyte with the release of oxygen. These are different processes that take place at the electrodes, compared to a standard solid oxide fuel cell, and the materials need to be optimised accordingly. One of the current challenges is how to have significant water incorporation at the electrodes. To achieve this, the material composition needs to be modified accordingly. Identifying new material structures may be difficult but developing composite materials with the right thermal expansion coefficient may be a more viable alternative.

In the short-term, materials research is very important to improve the durability of these devices. Initially, the research focus can be on traditional materials having traditional structures for example, perovskites or fluorites but with a tailored composition to obtain the right properties. Furthermore, materials research on the electrolytes, electrodes and interfaces is also important. The degradation of the existing materials is impacted by the transport across the interfaces so understanding and improving interfaces and interfacial transport is critical. Standardising test protocols to ensure that the results obtained by different research teams are comparable is also necessary to eliminate unpromising research routes.

Modelling and simulation approaches to materials development and deployment is also necessary. There is scope to work closely with theoretical scientists to accelerate the identification and development of candidate materials or systems, with engineers to consider cell, stack and system design, followed bydynamic modelling of devices in operation.

The engineering and manufacturing challenges of these new devices should also be considered. Current SOEC devices have planar designs, while their early stage generations were tubular. Producing hydrogen for certain applications, for example, *via* co-electrolysis for chemical feed stocks at pressure, may require tubular designs. This will impact the manufacturing process, the choice of materials, the scalability of technology and, ultimately, the final product price.

In the medium-term, the development of new materials that could be fundamentally different to the current options may be required. Integration of these materials in devices and manufacturing larger units will also be essential.

There is an urgent need to understand the fundamental factors that influence durability, in order to be able to develop products with lifetimes of ten years or more. Currently, SOFC stacks have demonstrated operation for several years and exhibit good reliability and lifetimes. For SOEC devices, the data are very limited, although these devices appear to operate well for one to two years. [99] The degradation mechanisms for fuel cell operation and electrolysis may be different so fundamental research in this area would be very valuable. Understanding the failure mechanisms *in operando* is necessary, although this is extremely challenging for ceramic devices that are operating at high temperatures (600 °C) .[100] Understanding long-term degradation is particularly difficult, as it may involve very slow processes, so is likely to require very sensitive analytical methods. The fundamental understanding of how failure modes occur and what the degradation processes are, need to be coupled with lifetime prediction and accelerated testing protocols for both high-temperature electrolysers and high-temperature fuel cells.

The US Department of Energy (DOE) estimates the energy efficiency for high-temperature electrolysers to be around 39 kW/h per kilogram of hydrogen. The target is around 43 kW/h per kilogram of hydrogen, corresponding to 10% of losses of the thermodynamic requirement. [101] The current degradation rate is therefore of the order of mV per year, which is encouraging. There is an issue of balancing the capital and running costs, where the running costs are dominated by the electrical energy cost. So, there is a need to optimise the current density at which these devices operate. Higher current densities may produce higher potential gradients, which would lead to enhanced rates of ionic migration in the electric fields and accelerated degradation. Modelling of these phenomena would be helpful to optimise and synchronise both the scientific and engineering developments required.

The UK scientific base in this area is strong, but industrial partnerships, especially for scaling up and manufacturing the technology should be supported further. Ideally, there should be an integrated programme involving both industry and academia to progress both technical and commercial developments for high-temperature electrolysers. This is currently somewhat hindered, as there is no large or mature industrial sector in this domain with sufficient commercial pull. Most companies involved are small, high technology, innovative businesses although large, industrial players are getting increasingly interested in this space.

Specific competencies on how to integrate high-temperature electrolysers with industrial processes would also be helpful, particularly in areas which are difficult to decarbonise, processes such as NH_3 synthesis, steel or cement production.[102,103]

The current deployment of this technology is very small, less than 0.1% of total H_2production. There have been some demonstration programmes, but no commercial H_2 production product as yet. If a global manufacturing and supply chain for the technology could be established that can deliver a commercial product with acceptable performance and lifetime, the uptake of this technology is likely to be very significant. Future deployment could be enhanced by focusing on specific geographical locations that have readily available electricity and heat generation. [104]

Government support, namely pricing CO_2 emissions to make this technology cost-competitive with established methods such as steam methane reforming, will also be needed.

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[99] Technical University of Denmark, Department of Energy Conversion and Storage 'E2P2H2 - 64013-0583 - Final report; Energy Efficient Production of Pressurized Hydrogen' 2016, https://energiteknologi.dk/sites/energiteknologi.dk/files/slutrapporter/e2p2h2_final_report_-_201600330.pdf

[100] R.J. Woolley, R.J *et al.* ' In Situ Measurements on Solid Oxide Fuel Cell Cathode- Simultaneous X-ray Absorption and AC Impedance Sectroscopy on Symmetrical Cells' Fuel Cells 13, 2013, 1080-1081 DOI: 10,1002/fuce.201300174

[101] US Department of Energy: The Hydrogen and Fuel Cell Technologies Office 'DOE Technical Targets for Hydrogen Production from Electrolysis' 2015, https://www.energy.gov/eere/fuelcells/doe-technical-targets-hydrogen-production-electrolysis

[102] https://www.green-industrial-hydrogen.com

[103] https://www.ammoniaenergy.org/wp-content/uploads/2019/12/NH3-Energy-2017-John-Hansen.pdf

[104] Staffell, I., *et al.*, 'The role of hydrogen and fuel cells in the global energy system' Energy Environ. Sci., ,12, 2019, 463-49, https://doi.org/10.1039/C8EE01157E .

The UK has a number of concentrated industry hotspots that would be able to integrate this technology into their industrial processes to create industrial symbiosis, although skilled process engineers to integrate and scale-up this technology will be required to achieve this. The electrolyser market could be larger than the fuel cell market, so focusing development time on this area could be very rewarding. This technology can also add value to existing renewable technologies for example by combining hydrogen and wind power.

Table 8 (below) shows the roadmap and the current and future performance requirements for this topic.

Table 8: Roadmap for the high temperature electrolysis: improve electrode and electrolyte materials topic

<table>
<tr><td>What is in scope</td><td colspan="5">Scalability and durability are important challenges.
Dynamic response time to load demand.
Are the properties of currently deployed materials for fuel cells effective at volume and scale for electrolysis?
Is there an appropriate material set used for fuel cells to be deployed for electrolysis. Can you make them work better? What is the best route for a range, for example, 1MW electrolyser?
It is important to capture for what hydrogen is used. Application and demand will set the targets. Hydrogen application is important; for example, for volume and low-cost demand there are different targets than feedstock.
Scale and device are important for industry; the scale depends on the industry it is used for, and where it will be used, for example, steam generation.
The technology is better when integrated with other processes.
It has an opportunity for integration with power generation and CO_2 capture.</td></tr>
<tr><td>Link to challenges</td><td colspan="5">Hydrogen is not naturally occurring and takes energy to release. A critical issue is where the electricity to undertake electrolysis would originate from (C2).
Hydrogen is difficult to store and distribute (C3).
There is a need for grid scale storage solutions, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore, significant materials innovation and systems integration are required (C4).
Industrial sector (reforming, ammonia, minerals, etc.) (C6).
Carbon-Neutral Aviation Fuel (C7).
Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point (C9).
UK wide H_2 delivery network at appropriate H_2 purity for maximum impact for distributed systems (C12).</td></tr>
<tr><td rowspan="3">Anticipated impacts this topic may have on the targets by 2050</td><td colspan="5">Targets (to be achieved by 2050)</td></tr>
<tr><td>Efficiency %</td><td>Scalability potential to 1 TW</td><td>Durability</td><td>Recyclability (end of life)</td><td>Carbon Footprint $kgCO_2e/MWh$ (cradle-to-grave)</td></tr>
<tr><td>High efficiency is a strong characteristic of this technology</td><td>This is an important challenge
Dynamic response time to load demand</td><td>This is a key challenge. Voltage degradation of less than 0.5%/kh. [105]</td><td>Life cycle assessment comparing different H2 production technologies available see ref Mehmeti et al.</td><td>5.10 - 23.32 kgCO2eq/kg H2. Depends on the electricity source (grid vs wind). [106]</td></tr>
<tr><td rowspan="2">Current and future performance</td><td colspan="2">Current state of art</td><td colspan="3">Desired future. Key performance characteristics / parameters</td></tr>
<tr><td colspan="2">At the moment the technology is more mature at the small scale (<100kW). [107, 108]
SOC technology for fuel cells more mature than high temperature electrolysers</td><td colspan="3"></td></tr>
</table>

[105] Fang, Q., *et al.* 'Performance and Degradation of Solid Oxide Electrolysis Cells in Stack' Journal of The Electrochemical Society, Volume 162, Number 8 2015 https://doi.org/10.1149/2.0941508jes
[106] Mehmeti, A. *et al.* 'Life Cycle Assessment and Water Footprint of Hydrogen Production Methods: From Conventional to Emerging Technologies'. Environments, 5, 24, 2018. https://doi.org/10.3390/environments5020024 .
[107] Yan, Z., *et al.* 'Renewable electricity storage using electrolysis', Proceedings of the National Academy of Sciences, 117 (23) 2020 12558-12563, DOI: 10.1073/pnas.1821686116.
[108] https://www.green-industrial-hydrogen.com

	Short-Term 2020 - 2025	Medium-Term 2025 - 2035	Long-Term 2035 - 2050
Technology Research and development path towards the desired future. Key milestones.	• Durability depends on materials • Traditional materials/structure fluorites, but the key point is the composition • Transport on interfaces • How to modify the composition, so the water incorporation process is significant • How to optimise the materials for both sub-processes • A composite material • Devices and operations modelling and simulation approaches for material development; engagement with theoretical scientists required; fluid dynamic models exist for fuel cells; but different models are needed for electrolysers • Associated with degradation, lifetime and durability is the *in situ, operando* testing, which is challenging at high temperatures • Research on chemical and interfacial characteristics; also, CO_2 environment • Lifetime prediction and accelerated testing; applies to high-temperature electrolysers and fuel cells • Trade-off between capital costs and operation costs; there is a requirement to optimise; modelling is required here; doing science and engineering in parallel, and not only in theory – integration of materials and devices, to understand where the issues in development are • Development of test protocols is necessary to make different results comparable and benchmark outcomes to have an indication of what should be taken forward • How to deal with the hydrogen produced • Production of hydrogen needs to be aligned with the location of the demand (market) **Manufacturing:** • Current SOEC are planar • If larger units are needed, how should the materials integrate? • Electrolyser market can be larger as fuel cell market	• Developing new materials and their manufacturing requires new processes • Fundamental understanding of factors that impact lifetime to 10,000 hours or more (for fuel cells: Sunfire (company in Germany) have run for more than a couple of years, 1–2y) • Modelling and simulation approaches for material development • DOE target 43kWh/kg hydrogen – losses will be 10% of thermodynamic (currently Sunfire achieves 38kWh/kg)[109] • Efficiency is the main advantage of SOEC, and its integration with industrial processes in the most efficient way, and this is how the technology should be driven towards the commercialisation; integration with low heat available where hydrogen can be used as feedstock	• How to decarbonise ammonia production • Decarbonisation and supporting of steel and cement production • Coupling of electrolysis with the above (currently requires high amount of electricity)[108]
Required competences and resources (finance,	• Combination of strong science base and partnership with industry for scale-up and	• The chemical market will be different by two orders of	

[109] US Department of Energy: The Hydrogen and Fuel Cell Technologies Office 'High Temperature, High Pressure Electrolysis; FY 2016 Annual Progress Report' 2016 https://www.hydrogen.energy.gov/pdfs/progress16/ii_b_4_mittelsteadt_2016.pdf

people, knowledge, partnerships etc.)	manufacturing; so, company can be involved in early-stage development; also, for development of the technology as an integrator • Interest is growing in investing in the topic, recruitment and infrastructure; there is also interest in operating this technology in reverse mode; but currently, it is not a large, mature industrial sector	magnitude (lower) than the energy market • Establish a global supply chain that has to meet cost requirements, but high promise by the efficiency • Consideration of the geographical location of hydrogen production; for example, it would be cheaper if located next to nuclear power plants	
Expected deployment (%) (linked to 1TW installed capacity)	**<0.1%** **(there are some demonstration programmes, but a fully commercial deployment)**		
Technology enablers	• Simulation tools to discover new materials *in silico* – key to accelerating material discovery (R1) • Analytical techniques for driving real understanding of the conversion processes, allowing us to "see" what's going on in real time; generating understanding of processes for optimisation (R2) • Efficient reactor designs for various chemistries (R6) • Fundamental surface science of, for example, electrolysis, catalysis, steam reforming, the processes that make hydrogen (R8) • Better understanding of reaction/degradation mechanisms (R11) • Wind power, hydroelectric, solar cells, and so on (renewables) (R15) • Device and system design and manufacturing (R16) • Experimental materials discovery assisted by computation (R17)		
Commercial enablers	• Price of carbon emissions in the future • Finding market and industrial processes where SOEC can be coupled to benefit from potential high efficiency • Hotspots of concentrated industry that could be integrated with this technology • Skilled engineers to operate (especially for large scale, the operation is a complex process), but in general skills are a broader issue; critical skill required is process engineering, which is important for integration • Capacity rather than availability of the right material is important for the growth of the new sector • Global partnerships to make capital available for small companies • Add value to existing renewable technologies, for example, adding value for wind energy generation by a new demand sink		

TOPIC 4: DIRECT PHOTOELECTROLYSIS (HE30): IMPROVE LIGHT ABSORBERS AND CATALYST MATERIALS

This topic focused on photoelectrochemical (PEC) / photocatalytic (PC) water splitting. Direct photoelectrochemical/photocatalytic water splitting is attracting extensive attention, with 100 m^2 photocatalytic demonstration plants already operational in Japan. Cost projections suggest that, with improved efficiency, some technologies could be cheaper than PV plus electrolysis. Photocatalytic systems in suspensions or sheets are highlighted for their opportunity for lower-cost production of hydrogen. Photoelectrochemical approaches with electrodes generally have higher efficiencies, but it is much more difficult to reduce their costs. Projections of the photocatalytic water-splitting method suggest they can be reasonably low cost, although there are challenges around the efficiency, durability and recycling.

There is a broad range of potential candidate materials in this area, both radical, and more standard, such as metal oxides for light absorbers and materials for catalysis, with opportunities for further discovery of suitable materials. There are several synergies in catalysis materials with electrocatalysis (c.f. Topics 1A and 6) and also in light absorber materials with photovoltaics (PV). Opportunities were noted with photoelectrochemical/photocatalytic CO_2 reduction and oxidative photoreforming processes (the oxidative synthesis of higher-value chemicals), with the latter potentially offering shorter-term commercial opportunities.

Catalysis and integrated system development are critical elements for both this topic and other priority topics in this domain. There are strong synergies between electrocatalysis and photosystems and how to integrate the catalysis into light absorbers and systems.

Regarding the technology readiness level, there are already small-scale demonstration devices elsewhere in the world, but these are lacking in the UK, so this is clearly a major motivation.

Many of the required competencies and resources are similar to some of the other areas, particularly electrocatalysis. In the medium-term, there is the opportunity for demonstration, particularly for demonstrating potential beyond hydrogen synthesis (for example, using both the H_2 and O_2 generated by water splitting).

A particular competence challenge, not specifically related to materials, is around the system engineering and scaling, which will become important as this technology scales up. In the long-term, the ambition would be to have both distributed micro generation and large-scale photocatalytic farms splitting water and synthesising H_2, but also potentially sustainable fuels and chemicals.

The expected deployment in terms of terawatts is probably less than 1% in the medium-term, but this could quickly scale up in the long-term. Scaling up will require availability of land and materials, as is the case with photovoltaics plus electrolysis.

Critical technological enablers are advances in electrocatalysis and PV materials. For this technology to be commercialised EPSRC and the UK Government will need to establish a clear and strong strategy. Aligning these activities with the catalysis group with the Catapult would also be helpful as well as combining both electro- and photoelectrocatalytic systems.

Table 9 (below) shows the roadmap and the current and future performance requirements for this solution.

Table 9: Roadmap for direct photoelectrochemical/photocatalytic water splitting: improve light absorbers and catalyst materials topic

<table>
<tr><td>What is in scope</td><td colspan="5">Interest in multiple metal oxides, inorganic nitrides/sulphides, perovskites, semiconducting polymers, Carbon Nitrides as light absorbers.
Inorganic and molecular catalysts, Catalysts discovery and optimisation.
Integration of catalysts and light absorbers into devices and systems; nanoscale engineering.
The system overall (extraction to recovery), solar collectors, non-toxic components.
Modelling for materials search prediction and whole system design.
Inspiration from natural systems.</td></tr>
<tr><td>What is out of scope</td><td colspan="5">Nothing, presently, but some materials will be displaced.</td></tr>
<tr><td>Link to challenges</td><td colspan="5">Public perception and education (C1).
Hydrogen is not naturally occurring and takes significant energy to release; therefore, as for PV + electrolysis, large scale H_2 generation will require large areas, and low- cost / m^2 – typically estimated as <$100/m^2 (C2).
Hydrogen is difficult to store and distribute (C3).
There is a need for grid scale storage solutions, and an integrated energy network linking electricity generation, storage, hydrogen production and storage; therefore, significant materials innovation and systems integration are required (C4).
Industrial sector (reforming, ammonia, minerals, etc.) (C6).
Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point (C9).
Subsidies to ensure competitiveness (C11).</td></tr>
<tr><td rowspan="3">Anticipated impacts this topic may have to the targets by 2050</td><td colspan="5">Targets</td></tr>
<tr><td>Efficiency %</td><td>Scalability potential to 1 TW</td><td>Durability</td><td>Recyclability (end of life)</td><td>Carbon Footprint kgCO$_2$e/MWh (cradle-to-grave)</td></tr>
<tr><td>PEC water splitting, 12%

PC water splitting, from 1% to 10% is possible
4x lower cost the PEC</td><td>PEC possible

PC possible</td><td>Stable materials tend to be lower durability; some progress on self-healing catalysts (e.g. CoPi)

Target of > 10-year lifetimes</td><td>Relatively unexplored.

Some components (e.g. catalysts) can be replaced to rejuvenate devices.</td><td>Potentially very low CO_2 emission; biggest challenges are emissions during metal extraction and material synthesis</td></tr>
<tr><td rowspan="2">Current and future performance</td><td colspan="2">Current state-of-the-art</td><td colspan="3">Desired future. Key performance characteristics / parameters</td></tr>
<tr><td colspan="2">PEC systems reported with efficiencies > 15%[110] but only with high cost and / or low durability; efficiencies of 3 % reported for lower cost materials (e.g. oxides).[111]

PC systems reported with efficiencies of 1-3% with low cost processing. Stable, large devices reported with efficiencies 0.1-0.5%.</td><td colspan="3">>10% conversion efficiencies with cost < $100 / m^2, 10-20-year stability and Earth abundant materials

Note: we have to consider the engineering of materials into systems.</td></tr>
<tr><td></td><td colspan="2">Short-Term
2020 - 2025</td><td colspan="2">Medium-Term
2025 - 2035</td><td>Long-Term
2035 - 2050</td></tr>
<tr><td>Technology research and development path towards the desired future. Key milestones.</td><td colspan="2">Optimisation of performance and stability with established materials.

Materials discovery.

Small-scale demonstration of devices.</td><td colspan="2">New earth abundant at 5% PC.

Additionality (beyond only H_2).

Demonstration-scale facilities, (H_2, O_2, other base stocks).</td><td>Large-scale PC farms generating E and PC splitting, feed to H_2 grids and sustainable fuels, chemicals.</td></tr>
<tr><td>Required competencies and resources (finance,</td><td colspan="2">Modelling across length scales.</td><td colspan="2">System engineering and scaling.</td><td></td></tr>
</table>

[110] Cheng, W.H., *et al.*, 'Monolithic Photoelectrochemical Device for Direct Water Splitting with 19% Efficiency' ACS Energy Letters, 3 (8), 2018, Pages 1795-1800, DOI: 10.1021/acsenergylett.8b00920.
[111] Pan, L., *et al.* 'Boosting the performance of Cu2O photocathodes for unassisted solar water splitting devices'. Nat Catal 1, 2018, Pages, 412–420. https://doi.org/10.1038/s41929-018-0077-6

people, knowledge, partnerships, etc.)	Materials discovery. *Operando* characterisation. Technology demonstration. Synthesis and scale. Biological science e.g. for bio-hybrid approaches		
Expected deployment (%) (linked to 1TW installed capacity)			
Technology enablers	• Simulation tools to discover new materials *in silico*; this is key to accelerating material discovery but requires materials design requirements (R1) • *Operando* analytical techniques for driving real understanding of the conversion processes, allowing us to "see" what's going on in real time; generating understanding of processes for optimisation (R2) • Identification of active catalyst states and catalytic mechanisms (R3) • Hybrid water-splitting techniques and chemical looping (R4) • Fundamental surface science of, for example, electrolysis, catalysis, steam reforming, the processes that make hydrogen (R8) • Better understanding of reaction mechanisms (R11) • Reduced or even non-precious metal content catalyst layers for PEMWE (R13) • Wind power, hydroelectric, solar cells, and so on (renewables) (R15)		
Commercial enablers	• Catalyst Catapult. • HMG industrial strategy (e.g. ISCF)		

TOPIC 5: THERMOCHEMICAL SYNTHESIS OF CHEMICAL FEEDSTOCKS: MATERIALS THAT ENABLE THE PRODUCTION OF CHEMICAL FEEDSTOCKS AT LOW PRESSURES AND TEMPERATURES (HI48&50&53)

This topic explored the use of hydrogen for the sustainable synthesis of chemical feedstocks, including ammonia, CO, methane, methanol, acetic acid, higher oxygenates (alcohols, DME) and hydrocarbons (olefins, aromatics, gasoline-type blends and aviation fuel). The materials challenges include new materials for solid oxide-based electrolysis for chemicals manufacture, catalysts for efficient conversion processes.

Direct methods, as well as tandem catalysis schemes, can be envisioned as using H_2 as a chemical feedstock. The reverse water gas shift reaction (which produces CO from CO_2) offers a good platform for bridging CO_2 utilisation with Fischer-Tropsch synthesis (which uses CO and H_2 as feedstock). Tandem catalysis strategies can include coupling RWGS with FT and coupling methanol synthesis from CO_2 with MTO processes. These stepwise conversions can also be performed in separate reactors using catalysts with already high TRLs in the short-term.

NH_3 synthesis *via* current Haber Bosch results in 1% of all CO_2 emissions[112]. Most of the CO_2 emissions could be avoided by replacing the current hydrogen production step of ammonia synthesis (steam reforming of methane) to renewable electricity-driven electrolysis (see Topics 1 and 2). Lowering the pressure required for ammonia synthesis would allow for decentralised NH_3 production. In this section, we focus on the distributed synthesis of NH_3 and identify the associated materials challenges: these are the development of catalysts that operate at low pressures and can be coupled with renewable hydrogen; oxygen-tolerant schemes avoiding the need for air separation; and the development of membranes for air separation in mild conditions.

Thermochemical methods of methanol production rely on high pressures, high temperatures and a largely CO-rich feed. While the use of CO_2 as feedstock for methanol synthesis is possible using existing technology and has been performed in some facilities (the largest being the George Olah Methanol synthesis plant in Iceland), commercial catalysts for methanol production are known to encounter kinetic limitations in additions to poor stability in CO_2-rich feeds. This ties into some of the materials challenges in this domain, such as the need for better catalysts for methanol production. In particular, for methanol production the catalysts used should be tailored to CO_2 hydrogenation, with suppression of the competing RWGS reaction [113,114,115,116], improved activity at high concentrations of CO_2 and extended stability in the presence of CO_2 and water. InO_2 and MoP catalysts are examples of this approach.

The thermochemical methods of CO_2 conversion and NH_3 synthesis are already efficient, and could be adapted to utilise hydrogen produced from renewables.

Regarding the required technological enablers, there is heavy emphasis on developing ways to characterise materials at different scales under dynamic conditions. Community-wide benchmarking testing protocols are critical for achieving many of the catalyst goals. Improved theoretical descriptions of catalysis of ammonia synthesis and CO_2-reduction reactions is also

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[112] The Royal Society 'Ammonia: zero-carbon fertiliser, fuel and energy store' Policy Briefing 2020 https://royalsociety.org/-/media/policy/projects/green-ammonia/green-ammonia-policy-briefing.pdf
[113] Studt, F., *et al.*, 'Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol'. Nature chemistry 6, no. 4, 2014, Pages 320-324. https://doi.org/10.1038/nchem.1873
[114] Duyar, M.S., *et al.*, 'Low-pressure methanol synthesis from CO_2 over metal-promoted Ni-Ga intermetallic catalysts' Journal of CO2 Utilization 39 2020 DOI: 10.1016/j.jcou.2020.03.001
[115] Gallo, A., *et al.*, 'Ni5Ga3 catalysts for CO2 reduction to methanol: Exploring the role of Ga surface oxidation/reduction on catalytic activity'. Applied Catalysis B: Environmental 267, 2020, 118369. DOI: 10.1016/j.apcatb.2019.118369
[116] Irek, S., *et al.*, 'Intermetallic compounds of Ni and Ga as catalysts for the synthesis of methanol' Journal of catalysis 320, 2014 Pages 77-88 https://doi.org/10.1016/j.jcat.2014.09.025 .

critical. There might also be a need to develop new materials that can purify air to remove O_2 and extract N_2 and CO_2. Especially in the case of NH_3 synthesis, materials development for distributed synthesis of products, it is possible that just feedstock purification or product purification would also be needed. [117]

Table 10 (below) shows the roadmap and the current and future performance requirements for this solution.

Table 10: Roadmap for the thermochemical synthesis of chemical feedstocks: materials that enable the production of chemical feedstocks at low pressures and temperatures topic

<table>
<tr><td>What is in scope</td><td colspan="5">• Hydrogen and hydrogen-related carriers
• Distributed processes
• Thermochemical ammonia synthesis coupled with renewable hydrogen
• Thermochemical CO_2 utilisation coupled with renewable hydrogen
• Catalyst discovery, development and membrane separation materials
• Solutions for geographies where the Haber-Bosch (H-B) process is expensive</td></tr>
<tr><td>What is out of scope</td><td colspan="5">Large scale, centralised Haber-Bosch processes (with the exception of thermochemical processes that can be completely renewably driven and operate at milder conditions)</td></tr>
<tr><td>Link to challenges</td><td colspan="5">• Hydrogen is difficult to store and distribute (C3)
• Industrial sector (reforming, ammonia, minerals, etc.) (C6)
• Carbon-Neutral Aviation Fuel (C7)
• Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point (C9)
• Subsidies to ensure competitiveness (C11)
• UK wide H_2 delivery network at appropriate H_2 purity for maximum impact (C12)
Additional key challenges:
• Needs to be competitive in relation to oil and gas
• Tax on fossil fuels
• Understanding of legislation around renewables</td></tr>
<tr><td rowspan="3">Anticipated impacts this topic may have to the targets by 2050</td><td colspan="5">Targets</td></tr>
<tr><td>Efficiency %</td><td>Scalability potential to 1 TW</td><td>Durability</td><td>Recyclability (end of life)</td><td>Carbon Footprint $kgCO_2e/MWh$ (cradle-to-grave)</td></tr>
<tr><td>Equilibrium methanol yield from CO_2 is 14% at 523K and 4MPa (stoichiometric H_2/CO_2)[118].</td><td>To be determined</td><td>To be determined</td><td>To be determined</td><td>Up to 1% of CO_2 emissions can be avoided by switching to renewable energy driven ammonia synthesis with green hydrogen.

90% drop in CO_2 emissions can be achieved by switching to CO_2 and renewable hydrogen as feedstock for methanol synthesis.

Carbon footprint is heavily tied to CO_2 emission per unit electricity. For completely renewable energy driven processes CO_2 hydrogenation becomes carbon consuming.</td></tr>
<tr><td rowspan="2">Current and future performance</td><td colspan="3">Current state-of-the-art</td><td colspan="2">Desired future. Key performance characteristics / parameters</td></tr>
<tr><td colspan="3">Oxygen tolerant schemes and catalysts have been demonstrated at lab scale for ammonia synthesis at mild conditions[119, 120].</td><td colspan="2">No ammonia in larger scale production as they may be heavy restrictions around the use of ammonia.</td></tr>
</table>

[117] Nilsson, A. & Stephens, I. E. L. in 'Research needs towards sustainable production of fuels and chemicals' (eds J.K. Nørskov, A. Latimer, & C. F. Dickens) 49 (Energy-X, Brussels, Belgium, 2019).
[118] Jiang, X., *et al.*, 'Recent Advances in Carbon Dioxide Hydrogenation to Methanol via Heterogeneous Catalysis' Chemical Reviews 120, 15, 2020 https://doi.org/10.1021/acs.chemrev.9b00723
[119] Rong, L., *et al.* 'Synthesis of ammonia directly from air and water at ambient temperature and pressure; Scientific reports 3, 1145, 2013, https://doi.org/10.1038/srep01145 .
[120] Rong, L., *et al.* 'Synthesis of ammonia directly from wet air at intermediate temperature' Applied Catalysis B: Environmental 152, 2014, Pages 212-217. https://doi.org/10.1016/j.apcatb.2014.01.037

	BASF/JM methanol production at 50-100 bar, 200-300 °C using SMR derived syngas (<10% CO2). 100 million tonne estimated market. <52% selectivity to methanol is reported with Cu-Zn catalysts in CO2 hydrogenation to methanol under similar conditions.[121] Methanol production from CO_2 and hydrogen at Carbon Recycling International facility in Iceland (George Olah plant) at 4000 tonne/year capacity. This plant is reported to achieve a 90% reduction in CO_2 emissions in comparison with fossil-based methanol synthesis.[122] CO_2 methanation is performed industrially (in ammonia synthesis) at 200-750 °C [123]. Power to gas applications are less established. Audi e-gas project in Germany operates at 300-400 °C, produces 1000 t/a synthetic natural gas, using hydrogen from 3 2MW alkaline electrolysers which operate during times of low electricity prices. Power to gas efficiency is reported as 54% and an 80% drop in CO_2 emissions is claimed for vehicles operating with e-gas instead of fossil fuels. [124] The EU Horizon 2020 "Store&Go" project has three demonstration sites, in Germany, Switzerland and Italy. Haber-Bosch operates at 400-500 °C and 150-250 bar, produces over 150 million metric tonnes of ammonia and consumes ~1% of the world's energy supply. It releases over 450 million metric tonnes of CO_2 annually. Electrochemical CO_2 reduction has been commercialised for CO production by Haldor Topsoe and Opus12. Electrochemical syngas generation is being used to supply a bioreactor in Rheticus II, a project by Siemens and Evonik for specialised chemical production from CO_2. This highlights the need for CO and syngas and the potential for implementing RWGS reactors in industry.	Ammonia -distributed electrochemical production coupled to renewables 1A/cm^2 and 50% efficiency. Low pressure methanol synthesis catalysts with higher stability in CO_2 rich conditions Methane –high mass activity catalysts operating at milder conditions in reactors that allow for optimised heat exchange (to manage exothermic reaction) and good turndown for variable operation in a power-to-gas scenario. Closed carbon cycle for using synthetic natural gas as renewables storage option. Replacing fossil fuels via production of sustainable fuels and chemicals from captured CO_2 and renewable hydrogen. For higher alcohol synthesis (HAS) via a CO intermediate (either tandem catalysis or separate reactors), targets are 90% selectivity to C2+OH and 60% single pass conversion according to NREL report on HAS. [125] FT catalysts achieve >70% single pass conversion, which is a relevant target for RWGS-FT schemes.

	Short-Term 2020 -2025	**Medium-Term 2025 -2035**	**Long-Term 2035 -2050**
Technology Research and development path towards the desired future. Key milestones.	Thermochemical methanol synthesis - lower-pressure and higher stability catalysts for CO_2 conversion. Thermochemical ammonia synthesis – lower-pressure ammonia synthesis catalyst,	Low temperature plasma catalysis for CO_2 and nitrogen reduction. [126],[127] Nitrogen reduction to other nitrogen-based compounds - not ammonia e.g. amides.	Catalyst materials for the direct conversion of CO_2 to any petroleum-derived products. Aviation fuel.

[121] Tackett, B.M., *et al.* 'Net reduction of CO_2 via its thermocatalytic and electrocatalytic transformation reactions in standard and hybrid processes' Nature Catalysis 2, 2019, Pages 381–386 https://doi.org/10.1038/s41929-019-0266-y

[122]The Royal Society, 'Sustainable synthetic carbon based fuels for transport' 2019. https://royalsociety.org/-/media/policy/projects/synthetic-fuels/synthetic-fuels-briefing.pdf

[123] The Oxrod Institute for Energy Studies, 'Power-to-Gas: Linking Electricity and Gas in a Decarbonising World?' 2018, https://www.oxfordenergy.org/wpcms/wp-content/uploads/2018/10/Power-to-Gas-Linking-Electricity-and-Gas-in-a-Decarbonising-World-Insight-39.pdf

[124] Otten, R., 'The first industrial PtG plant – Audi e-gas as driver for the energy turnaround' http://www.cedec.com/files/default/8-2014-05-27-cedec-gas-day-reinhard-otten-audi-ag.pdfhttp://www.cedec.com/files/default/8-2014-05-27-cedec-gas-day-reinhard-otten-audi-ag.pdf

[125] Phillips S, et al., Technical Report ' Thermochemical Ethanol via Indirect Gasification and Mixed Alcohol Synthesis of Lignocellulosic Biomas' US department of Energy, Office of energy effieciecy and rensewable energy 2007, https://www.nrel.gov/docs/fy07osti/41168.pdf

[126] Mehta, P., *et al.* 'Overcoming ammonia synthesis scaling relations with plasma-enabled catalysis' Nature Catalysis 1, no. 4, 2018, Pages 269-275. https://doi.org/10.1038/s41929-018-0045-1

[127] Mehta, P., *et al.* 'Catalysis enabled by plasma activation of strong chemical bonds: A review' ACS Energy Letters 4, no. 5, 2019, Pages 1115-1133. https://doi.org/10.1021/acsenergylett.9b00263 .

	materials for distributed air separation. Oxygen tolerant catalysts. CO_2 reduction to acetate and CO (possibly formats). CO_2 to liquid fuels and chemical feedstocks using RWGS+FT or CO_2 to MeOH + MTO-type processes.	Low-cost abundant materials for hybrid thermal-electrochemical-biological [128]methods for nitrogen reduction (also see Topic 6). [129] Tandem catalysts for converting CO2 to liquid fuels and chemical feedstocks.	
Required competences and resources (finance, people, knowledge, partnerships etc.)	Development of modular chemicals production prototypes that can be coupled with electrolysers. Engineering expertise and industry partnerships to reach demonstration scale. Demonstration of CO_2 consuming processes using existing concentrated sources of CO_2.	CO_2 capture and availability of hydrogen at point sources of emissions.	Demonstration scale chemicals production using CO_2 from air for negative emission distributed chemicals production.
Expected deployment (%) (linked to 1TW installed capacity)			
Technology enablers	• Ways to characterise materials. • Community-wide benchmarking testing protocols. • Developing the theory of materials catalysis. • Methods for handling large amounts of data for materials modelling. • Air-purification methods for ammonia synthesis at mild conditions or oxygen tolerant systems. • Benchmarking performance of catalysts under variable operating conditions and using renewable hydrogen sources.		
Commercial enablers	• Lowering the carbon footprint of hydrogen by increasing renewable electricity penetration into the grid. [130] • Lowering the cost of blue and green hydrogen to be competitive with grey hydrogen. • Deploying larger-scale electrolysers. • The use of renewable energy for CO_2 hydrogenation is critical for the net-reduction of CO_2 in methanol synthesis.[131] • Demonstrators - platform technology approach - synthesising chemical on a smaller scale will accelerate large scale uptake in the future. • Systems engineering.		

[128] McEnaney, J. M., *et al.* 'Ammonia synthesis from N_2 and H_2O using a lithium cycling electrification strategy at atmospheric pressure' Energy & Environmental Science 10, no. 7 (2017): 1621-1630. https://doi.org/10.1039/C7EE01126A
[129] Chong Liu, C., *et al.* 'Hybrid inorganic–biological nitrogen reduction' Proceedings of the National Academy of Sciences 201706371, 2017, DOI: 10.1073/pnas.1706371114
[130] https://hydrogencouncil.com/en/path-to-hydrogen-competitiveness-a-cost-perspective/
[131] Jiang, X., *et al.* 'Recent Advances in Carbon Dioxide Hydrogenation to Methanol via Heterogeneous Catalysis' Chemical Reviews, 120, 15, 7984–8034 2020, https://doi.org/10.1021/acs.chemrev.9b00723

TOPIC 6: ELECTROCHEMICAL REDUCTION OF CARBON DIOXIDE AND NITROGEN: DISCOVER CATALYSTS, ELECTRODES AND ELECTROLYTES YIELDING HIGH ACTIVITY AND SELECTIVITY (HC20)

This topic explored the development and use of better electrode and catalytic materials for electrochemical reduction, including CO_2 (CO_2 -RR) and nitrogen reduction (N_2-RR). The key issues with such processes are the catalyst stability and selectivity. The stability for molecular catalysts, selectivity and limited materials are major challenges. Stability and efficiency are issues for inorganic catalysts.[132]

The reduction of CO_2 and N_2 presents challenges because of the diversity of products that can be formed, particularly in the case of CO_2. The development targets should therefore target a high current density, high pass efficiency and high Faradaic efficiency, in terms of the desired products created (*e.g.* methanol, ammonia). In the case of H_2 production, potential efficiency of the catalyst is critical, whereas for applications such as CO_2 reduction, potential efficiency may be less critical than Faradaic efficiency, if there is a subsequent energetic cost to product separation for low specific Faradaic efficiencies; this is especially the case for high value products. In principle, electrochemical reduction processes are highly scalable, adapting some of the extensive knowledge gained from the hydrogen fuel cell/electrolyser fields, and electrolytic chlorine production but the specifics depend on the catalyst used. Catalysts and electrolytes are very much open (and highly topical) research questions for these systems. Regarding the CO_2 footprint and, in particular the CO_2-RR, any process will need to ensure that the carbon footprint is negative namely, that net carbon is taken out of the atmosphere to make a difference to national de-carbonisation targets.

The most extensively researched catalysts in the context of CO_2-RR are those based on copper.[133] Cu and its alloys are still the most promising materials for CO_2 reduction to methane, whereas Sn-based catalysts are the most extensively researched materials for formate production and Ag for reduction to CO.[134] CO_2 reduction to C_2 products, such as ethylene or ethanol, is also an important target. Again, Cu catalysts are at the fore here, with high current densities (1.3 A cm^{-2}) in alkaline aqueous solutions recently reported.[135] While conducting CO_2 reduction in alkaline solution may enhance catalysis, it results in poor CO_2 utilisation due to the reaction of CO_2 to form carbonates and bicarbonates.[136]

Catalyst (nano)-structure and electrolyser design have been shown to be key issues. In terms of electrolytes, it has been known for many years that protonated (formate, alcohols) products are more readily formed in aqueous solutions, whereas non-aqueous media more readily favour CO and oxalate formation. Recent works have explored “in vogue” materials in the CO_2-RR context, with materials such as MoS_2 showing promise, although the latter’s use appears to be restricted to ionic liquids, which would bring problems in terms of decomposition and cost.[137] There have also been many reports describing the use of supported molecular catalysts, such as metal phthalocyanine complexes, but here long-term stability/lifetime is likely to be a problem.

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[132] M. T. & Roldan Cuenya, B. in *Research needs towards sustainable production of fuels and chemicals* (eds J.K. Nørskov, A. Latimer, & C. F. Dickens) 49 (Energy-X, Brussels, Belgium, 2019).
[133] Nitopi, S., *et al.* ‘Progress and Perspectives of Electrochemical CO_2 Reduction on Copper in Aqueous Electrolyte’ Chem. Rev.119, 12, 2019, Pages 7610–7672, https://doi.org/10.1021/acs.chemrev.8b00705
[134] Liu, A.M., *et al.* ‘Current progress in electrocatalytic carbon dioxide reduction to fuels on heterogeneous catalysts’, J Mater. Chem A, 8, 2020, Pages 3541-3562, https://doi.org/10.1039/C9TA11966C
[135] Pelayo García de Arquer, F., *et al.* Science, 367 (2020), 661 https://science.sciencemag.org/content/367/6478/661.editor-summary
[136] Ma, M., *et al.* ‘Insights into the carbon balance for CO2 electroreduction on Cu using gas diffusion electrode reactor designs’ Energy Environ. Sci. 13, 977, 2020, https://doi.org/10.1039/D0EE00047G
[137]Andersen, S.Z., *et al.* ‘A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements’, Nature 570, 2019, 504–508, https://doi.org/10.1038/s41586-019-1260-x

For N_2-RR, the field is in its early stages and there is not really a clear, outstanding candidate catalyst for this system at the moment. Research therefore should focus on materials discovery, trying to find the best active catalysts. A recent Nature paper[138] indicated that there are false positives are prevalent amongst the current reports on N_2-RR electrocatalysts, resulting from the difficulties in using the relevant characterisation methods with the small quantities of "product" involved.In the future, CO_2 -RR research should be able to deliver high cell activity towards a high value or useful product, and relatively high Faradaic efficiency. In N_2-RR a successful outcome would be to identify an active catalyst.

The current state-of-the-art is based on the current performance metrics of ammonia synthesis electrocatalysts, which are 2% current efficiency at 70 mA cm^{-2}.[139,140,141]

In terms of technology readiness, N_2-RR is not as mature as CO_2-RR. The development of CO_2 -RR can now be said to have reached a stage where devices could be built, moving onto prototype reactors in the medium-term and actual deployment in the long-term. The development of N_2-RR is further behind, where a suitable catalyst(s) needs to be identified before prototype devices in and prototype reactors could be built in the medium and long-terms, respectively.

In terms of the competencies needed, robust electrocatalytic benchmarking is a key requirement, in addition to *in operando* characterisation of the operation of those catalysts. The comparison of different catalysts should be done robustly to eliminate false positives. In the UK, more people should be trained and employed in electrocatalysis. Academic engagement with the oil and gas industry, in particular, should be used to develop partnerships with energy suppliers and enable scale-up/technology transfer.

In the medium-term the whole supply chain needs to be developed, and, in the long-term, remediation of spent catalysts needs to be considered.

The anticipated deployment for this technology was defined as the percentage production versus other ways of making ammonia and hydrocarbons, respectively, for N_2-RR and CO_2-RR. Currently, both technologies are under development and therefore at 0% deployment, although some start-ups have appeared recently in the CO_2-RR sector (see Topic 5). The expectation is to be able to achieve approximately 40% deployment of CO_2 -RR in the long-term, recognising that there are other routes to increasing hydrogen production, such as thermochemical routes (again, see Topic 5). In the longer term, the N_2-RR method has the potential to be deployed for decentralised, small-scale ammonia production, where capital costs may be a constraint and where the efficiencies of centralised Haber-Bosch production cannot be realised. This could include the ability to prepare fertiliser feedstock at remote locations where the conventional (Haber-Bosch) routes are inaccessible because of the transport costs (although this driver may be less relevant in the UK context). This may account for up to 10% of production by 2050.

Table 11 (below) shows the roadmap and the current and future performance requirements for this solution.

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[138] Andersen, S.Z., *et al.* 'A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements', Nature 570, 2019, 504–508, https://doi.org/10.1038/s41586-019-1260-x
[139] Tsuneto, A., et al. 'Lithium-mediated electrochemical reduction of high pressure N2 to NH3' Journal of Electroanalytical Chemistry, 367 1994, Pages 183-188 https://doi.org/10.1016/0022-0728(93)03025-
[140] Lazouski, N., Chung, M., Williams, K. et al. Non-aqueous gas diffusion electrodes for rapid ammonia synthesis from nitrogen and water-splitting-derived hydrogen. Nat Catal 3, 2020, 463–469. https://doi.org/10.1038/s41929-020-0455-8
[141] Andersen, S.Z., *et al.* 'A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements', Nature 570, 2019, 504–508, https://doi.org/10.1038/s41586-019-1260-x .

Table 11: Roadmap for the electrochemical reduction of carbon dioxide and nitrogen: discover catalysts, electrodes and electrolytes yielding high activity and selectivity topic

What is in scope	**CO_2-RR:** Copper Nano Particles; Nano Structuring of surfaces; Surface activation with plasma using N and O; Electro-chemical nano-structuring; **N_2-RR:** New material discovery
What is out of scope	**N_2-RR:** Numerous proposed catalysts not effective[142]
Link to challenges	• There is a need for grid scale storage topics, and an integrated energy network linking electricity generation, storage, hydrogen production and storage; therefore, significant materials innovation and systems integration are required (C4) • Carbon-neutral aviation fuel (C7) • Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point (C9) • Development of Carrier Distribution Network (C10)

	Targets				
	Efficiency %	**Scalability potential to 1 TW**	**Durability**	**Recyclability (end of life)**	**Carbon Footprint $kgCO_2e/MWh$ (cradle-to-grave)**
Anticipated impacts this topic may have to the targets by 2050	Faradaic efficiency = 70%; for large scale applications, energy efficiency is also important for minimising the overall cost of fuels as electricity will be a large component	High (100%) achievable provided catalyst is abundant	10 years of catalyst lifetime	Important if rare; 60-80% catalyst recovery	Less than 0

	Current state-of-the-art	**Desired future. Key performance characteristics / parameters**
Current and future performance	**CO_2-RR:** Copper based catalysts; Gold Nano Particles; MoS_2 Catalyst; Molecular Catalyst; Transition metal catalysts; Cobalt Phthalocyanine; pyridine and transition metal complexes of pyridines; 3 V, 100 hrs lifetime, high (>95%) overpotential for simplest reduction products (CO and formate)[143] **N_2-RR:** 2.8% electricity to ammonia efficiency at partial current density of 9 mA cm^{-2} using lithium mediated route. [144-145]	**CO_2-RR:** High selectivity towards high value/useful products; efficiency; Electrochemical CO_2 reduction - stable cell voltage of around 2V and >90% efficiency to ethylene 2A Acetic acid - low cost catalyst for electrodes and increased conversion efficiency, durability > 10k hours **N_2-RR:** **i**dentifying an active catalyst; widespread deployment capability; Ammonia - distributed electrochemical production coupled with renewables $1A/cm^2$ and 50% efficiency

	Short-Term 2020-2025	Medium-Term 2025-2035	Long-Term 2035-2050
Technology Research and development path towards the desired future. Key milestones.	**CO_2-RR:** getting on TRL 2-3; build critical mass for the UK CO_2 RR activity; Prototype Reactors TRL 4-5; There are already prototype reactors and companies commercialising CO_2 reduction[146]. **N_2-RR:** TRL 1-2; identify any active catalyst;	**CO_2-RR:** prototype reactors for making an impact to overall emissions, ultimately large volume chemicals need to be targeted, such as ethylene or fuels like ethanol; for achieving zero emissions by 2050, CO_2-negative technologies are needed, for instance using CO_2 to make materials that will not get burnt back to CO_2 eventually (e.g. materials for construction).	**CO_2-RR:** Field deployment for CO and formate; lifetime increase to 100,000 hrs Faradaic efficiency (at scale) > 70% for more complex (alcohols, C2) products. **N_2-RR:** Prototype Reactor. N_2 follows behind CO_2 development

[142] Andersen, S.Z., *et al.* 'A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements', Nature 570, 2019, 504–508, https://doi.org/10.1038/s41586-019-1260-x
[143] Koper, N., and Cuenya, B.R., 'Research needs towards sustainable production of fuels and Chemicals; Chapter 2 Electochemical CO_2 Reduction' Edited by Nørskov, J.K., 2019 https://www.energy-x.eu/wp-content/uploads/2020/02/Energy_X_Research-needs-report_final_24.02.2020.pdf
[144] Andersen, S.Z., *et al.* 'A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements', Nature 570, 2019, 504–508, https://doi.org/10.1038/s41586-019-1260-x
[145] Lazouski, N., Chung, M., Williams, K. et al. Non-aqueous gas diffusion electrodes for rapid ammonia synthesis from nitrogen and water-splitting-derived hydrogen. Nat Catal 3, 2020, 463–469. https://doi.org/10.1038/s41929-020-0455-8
[146] Haldor Topsoe make CO using solid oxide electrolysers. Opus 12 does it at low temperatures: https://www.opus-12.com/about

		N_2-RR: devices TRL 2-3;	Electrochemical synthesis of ammonia (direct from water and nitrogen) Catalyst material, electrolytes and other interfaces CO_2 to any petroleum derived products Aviation fuel
Required competences and resources (finance, people, knowledge, partnerships etc.)	Robust electro-catalytic benchmarking mechanisms; More people in UK working in electrocatalysis; Industrial expertise; Partnership with electricity suppliers; Consultancies in energy sector; Oil industry to venture into the development; *Operando* characterisation	Supply chain optimisation; Partnerships with industry suppliers including oil and gas industry.	Circular supply chain dealing with catalyst; Remediation;
Expected deployment (%) (linked to 1TW installed capacity)	**CO_2-RR:** 0 % of hydrocarbon and oxygenate production (Deployment vs. Current measures of producing methanol and other hydrocarbons and oxygenates) **N_2-RR:** 0 % (deployment vs current measures of producing ammonia or others).	**CO_2-RR:** 10 % **N_2-RR:** 0 %;	**CO_2-RR:** 40 % **N_2-RR:** 10 %
Technology enablers	• Simulation tools to discover new materials *in silico*; this is key to accelerating material discovery (R1) • Analytical techniques for driving real understanding of the conversion processes, allowing us to "see" what's going on in real time; generating understanding of processes for optimisation (R2) • Identification of active catalyst state (R3) • Fundamental surface science of, for example, electrolysis, catalysis, steam reforming, the processes that make hydrogen (R8) • Better understanding of reaction mechanisms (R11) • Wind power, hydroelectric, solar cells, and so on (renewables) (R15)		
Commercial enablers	• Incentives and mechanisms • Small-scale widespread applications • Regulatory framework		

LINKING PRIORITY TOPICS TO CHALLENGES AND RESEARCH, TECHNOLOGIES AND ENABLERS

The priority topics were evaluated against the different challenges identified for the sector. The main purpose was to assess whether these challenges are addressed by the topics selected as priorities, or if there are any gaps, where additional work is required. The links between priority topics and challenges is shown in Figure 11 (below).

Challenges		Topic 1A: Proton Exchange Membrane (PEMWE) electrolysers: *Decrease or eliminate precious metals from catalysts*	Topic 1B: Proton Exchange Membrane (PEMWE) electrolysers: *Improve cost, stability and conductivity of electrode materials*	Topic 2: Alkaline electrolysers	Topic 3: Solid oxide electrolysers	Topic 4: Direct photocatalytic water splitting	Topic 5: Thermochemical synthesis of chemical feedstocks	Topic 6: Electrochemical reduction of carbon dioxide and nitrogen
C1	Public perception and education	■		■		■		
C2	Hydrogen is not naturally occurring and takes a huge amount of energy to release. A critical issue is where the electricity to undertake electrolysis would originate from.	■	■	■	■	■		
C3	Hydrogen is difficult to store and distribute.			■	■	■	■	
C4	There is need for grid scale storage topics, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore, significant materials innovation and systems integration are required.	■	■	■	■	■		■
C5	The main production technologies that produced reasonable volumes of compressed hydrogen are not practically scalable, and thus it is essential that alternatives are found.			■				
C6	Industrial sector (reforming, ammonia, minerals, etc.).		■		■	■	■	
C7	Carbon-neutral aviation fuel.	■			■		■	■
C8	Viable technologies.		■	■				
C9	Decarbonisation of chemical production, all industrial processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point.	■	■	■	■	■	■	■
C10	Development of carrier distribution network.							■
C11	Subsidies to ensure competitiveness.			■		■	■	
C12	UK wide H_2 delivery network at appropriate H_2 purity for maximum impact.		■	■	■		■	

	C13	Policy and regulation for hydrogen economy.							
	C14	Needs to be competitive in relation to oil and gas.							
	C15	Tax on fossil fuels.							
	C16	Understanding of legislation around renewables.							

Figure 11: Links between the priority topics and the domain challenges

In order to derive the key research priorities for hydrogen energy materials, participants were asked to summarise from the technology layer of each application roadmap the most important research activities.

In total, 25 research activities were put forward and assessed. From these, the following seven were selected as being important by most topics, indicating that their realisation and achievement would have a positive impact on several topics. These were:

- Simulation tools to discover new materials *in silico*. This is key to accelerating material discovery (R1).
- Analytical techniques for driving real understanding of the conversion processes, allowing us to observe real time processes. Generating mechanistic understanding leading to dsign optimisation (R2).
- Identification of active catalyst state (R3).
- Fundamental surface science of, for example, electrolysis, catalysis, steam reforming, the processes that make H_2 (R8).
- Better understanding of reaction mechanisms (R11).
- Reduced or non-precious metal content catalyst layers for PEMWE (R13).
- Wind power, hydroelectric, solar cells, and so on (renewables) (R15).

Therefore, supporting research activities in these areas would have a positive spill over effect on the overall development of this sector and aid the commercialisation of new technologies.

The links between the priority topics and research priorities were captured and assessed and they are shown in Figure 12 (below).

			Topic 1A: Proton Exchange Membrane (PEMWE) electrolysers: *Decrease or eliminate precious metals from catalysts*	Topic 1B: Proton Exchange Membrane (PEMWE) electrolysers: *Improve cost, stability and conductivity of electrode materials*	Topic 2: Alkaline electrolysers	Topic 3: Solid oxide electrolysers	Topic 4: Direct photocatalytic water splitting	Topic 5: Thermochemical synthesis of chemical feedstocks	Topic 6: Electrochemical reduction of carbon dioxide and nitrogen
Research, Technology, Enablers	R1	Simulation tools to discover new materials *in silico*. This is key to accelerating material discovery.							
	R2	Analytical techniques for driving real understanding of the conversion processes, allowing us to "see" what's going on in real time. Generating understanding of processes for optimisation.							
	R3	Identification of active catalyst state.							
	R4	Hybrid water-splitting techniques and chemical looping.							
	R5	Humidity capture for heat storage in hydrogen tank.							
	R6	Efficient reactor designs for various chemistries.							
	R7	Electrochemical hydrogen compression technologies.							
	R8	Fundamental surface science of, for example, electrolysis, catalysis, steam reforming, the processes that make hydrogen.							
	R9	Hydrogen-on-demand fuel tanks and fuel cell engines.							
	R10	Phase control for metallic TMD catalysts.							
	R11	Better understanding of reaction mechanisms.							
	R12	More efficient microbial systems for higher Cn compounds.							
	R13	Reduced or even non-precious metal content catalyst layers for PEMWE.							
	R14	Durable and active AEM membrane development.							
	R15	Wind power, hydroelectric, solar cells, and so on (renewables).							
	R16	Professional, independent facilities for short- and long-term *operando* testing (including synchrotron facilities and neutron imaging) and validation of new materials under relevant conditions. Imaging of catalyst layers *in situ* and *ex situ* testing.							
	R17	High throughput testing for new and novel catalyst motifs, including engaging with computational chemists.							

	R18	Partnerships: an interaction between academic and industrial partners who understand how things will operate in a stack and what the real need is, academics who can develop new materials and methods, and research institutes who can bridge the gap and support scale-up and testing, for example, Horizon 2020 projects in the UK.							
	R19	Facilities for *in operando* testing of catalysts.							
	R20	High throughput testing for catalysts. Imaging of catalyst layers *in situ* and *ex situ* testing (already done in fuel cells).							
	R21	Access to synchrotron facilities and neutron imaging.							
	R22	Table-top synchrotrons (groups in Korea and China working on these).							
	R23	Moving toward single-atom catalysts to reduce the amount of Pt and Iridium catalysts used.							
	R24	Device and system design and manufacturing.							
	R25	Experimental materials discovery assisted by computation.							

Figure 12: Links between the priority topics and the supporting research activities

CONCLUSIONS AND NEXT STEPS

Hydrogen is expected to be a significant contributor to the UK's 2050 decarbonisation targets. The development of materials and technologies to enable the wide adoption of low-carbon hydrogen in the UK's future energy is a critical activity for this ambition. Six priority **topics** were identified that have the potential to make step-changes in research to reach the UK's 2050 net-zero targets. These were as follows:

- Proton exchange membrane electrolysers
    - Decrease or eliminate precious metals from catalysts
    - Improve cost, stability and conductivity of electrode materials
- Alkaline electrolysers
    - Improve membrane stability and conductivity
    - Improve catalyst activity
- Solid oxide electrolysers
    - Improve electrode and electrolyte materials
- Direct photoelectrolysis
    - More efficient and stable photoelectrode and photocatalyst materials
- Thermochemical synthesis of chemical feedstocks
    - More efficient catalysts and other materials that enable the production of chemical feedstocks at low pressures and temperatures
- Electrochemical reduction of carbon dioxide and nitrogen
    - Discover catalysts, electrodes and electrolytes yielding high activity and selectivity

In conjunction with the research developments, several **commercial enablers** need to be established to accelerate the deployment and adoption of these technologies. These are:

- The capability and funding to manufacture materials, catalysts and systems on a large scale so that they can be commercially tested. This could be achieved in partnershipintegration with the **Catapult** network**.** Potentially, adventurous ARPA-type programmes for the UK in catalysis and energy materials.
- Access to **venture capital** and early **investment**, and global partnerships to make capital available **for small companies.**
- **British industrial champion(s)** that could drive forward the commercialisation of new technologies, as well as **hotspots of concentrated industry** that could be integrated with these technologies.
- **Well-resourced collaboration opportunities and support to such up relationships** within the UK between academia, industry, and research institutions, these could be facilitated with greater coordination and cooperation between the Henry Royce Insisute, the UK Catalysis Hub, H2FC Supergen, the Faraday Institution, etc.
- Strong collaboration with **international** partners and integration in international supply chains.

- Participation in international research funding programmes (*e.g.* Horizon Europe's forthcoming Sunergy programme).
- Cheap **access to renewable energy sources** (RES) exploiting the UK's large off-shore RES resources. This could enable hydrogen integration with the electricity grid, as well as utilising the UK's manufacturing capability, but it will require **government support** and an **updated regulatory framework that reflects the opportunities for net-zero afforded by the hydrogen economy**. For example, **regulatory, political and/or tax incentives**, such as a carbon tax for wide roll-out of the use of renewable energies to enable 100% green hydrogen generation. This will offer the flexibility of being able to produce hydrogen in both a decentralised and centralised manner, at different scales and with distributed or non-distributed generation.
- **Regulation to accelerate industrial industries**, for example, green hydrogen use in refineries.
- A **business case** that differentiates the benefits of producing hydrogen through electrolysis using renewable power sources (green hydrogen) from hydrogen produced from fossil fuels (blue hydrogen).
- **Identification of niche markets** and **industrial processes** for the electrolytic production of hydrogen and other related fuels and chemicals. Capacity rather than availability is important for growth of the new sector

Education enablers include:

- **Improved and new training opportunities to fill the hydrogen skills gap**, which is large in the UK.
- **Training of new electrochemical engineers and process engineers** to operate large-scale operations.
- **University curricula** that **raise awareness** of hydrogen and carbon-neutral fuels and feedstocks and the differences with the carbon positive equivalents used today
- **Alignment between universities and engineering bodies** (e.g. IChemE, IMechE, IEE, Energy Institute etc.) for university course accreditation schemes to promote and make attractive the uptake of these sustainable technologies.

There is a significant opportunity within the country to invest green hydrogen technologies[147] because the UK has one of the largest renewable electricity generating capabilities in Western Europe.

The **UK has a world-leading position** in this area. Further co-ordinated and targeted support would be helping both the UK's ambition for net zero by building a robust efficient, durable and sustainable hydrogen industry and providing economic potential for exporting technology and know-how to the rest of the world.

[147] Green hydrogen is hydrogen generated through electrolysis using electricity produced via renewable power sources

NEXT STEPS

Fundamental research in materials science, device fabrication and translation capability are urgently required to develop low-carbon hydrogen technologies. A key requirement for any technology development in this domain is having a sustainable and stable resource supply as well as end-of-life recycling options. For any existing or new materials used, improved recyclability and reactivation of materials will also be important for the sustainable, long-term use of these technologies. There is a compelling need to reduce future reliance on resource-limited or expensive critical materials, such as ruthenium or iridium.

These challenges will be addressed through enhancements in our understanding of electrocatalytic water oxidation, application of data- intensive learning techniques, and improvements in advanced manufacturing capability, leveraging the UK's investments in the research infrastructure alongside the extensive network of active SMEs in the hydrogen sector from across the UK.[8]

In addition, the development of appropriate scaling up facilities, changes in the regulatory framework and support for skills development would be important enablers for the commercialisation and adoption of these technologies. In particular, the following activities are considered very important for assisting the adoption of low-carbon hydrogen in the UK's energy system:

- Community-wide bench-marking **testing protocols;**
- Testing facilities of new materials in prototype devices at single cell level using device geometries intermediate between those available in academic institutions and in full electrolyser stacks;
- **Component development** for example, durable and conductive alkaline membranes
- Methods to improve the **recyclability and reactivation** of existing or new materials
- Development of a fundamental understanding of **reaction and degradation mechanisms;**
- **Ultra-sensitive analytical techniques**, which would allow us to observe reaction intermediates, desired reaction products and undesired side products, including corrosion products, over the short time scales of typical laboratory experiments;
- Advanced ***operando* and *ex situ* characterisation techniques**, strongly integrated with benchmark performance tests, to establish the characteristics of materials that are responsible for superior functionality;
- **Integrated experimental and computational programmes** where simulation tools both guide materials discovery and aid interrogation and interpretation of experimental data, for example, to predict new materials *in silico*, which is key to accelerating material discovery.

APPENDIX I: PARTICIPANTS

PARTICIPANT	AFFILIATION
Gerry Agnew	St Andrews University
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Diana Khripko	IfM ECS (Facilitator)
Imoh Ilevbare	IfM ECS (Facilitator)
Arsalan Ghani	IfM ECS (Facilitator)
Andi Jones	IfM ECS (Facilitator)
Rob Munro	IfM ECS (Facilitator)

Workshop Details

The workshop was commissioned by the Henry Royce Institute and delivered by Institute for Manufacturing, Education and Consultancy Services Limited.

Dates
First session: 20 March 2020, 10.00–12.00
Second session: 27 March 2020, 09.00–10.00
Third session: 27 March 2020, 13.00–15.00
Fourth session:01 May 2020, 14.00–16.00
Fifth session:05 May 2020, 14.00–16.00
Sixth session:14 May 2020, 14.00–16.00

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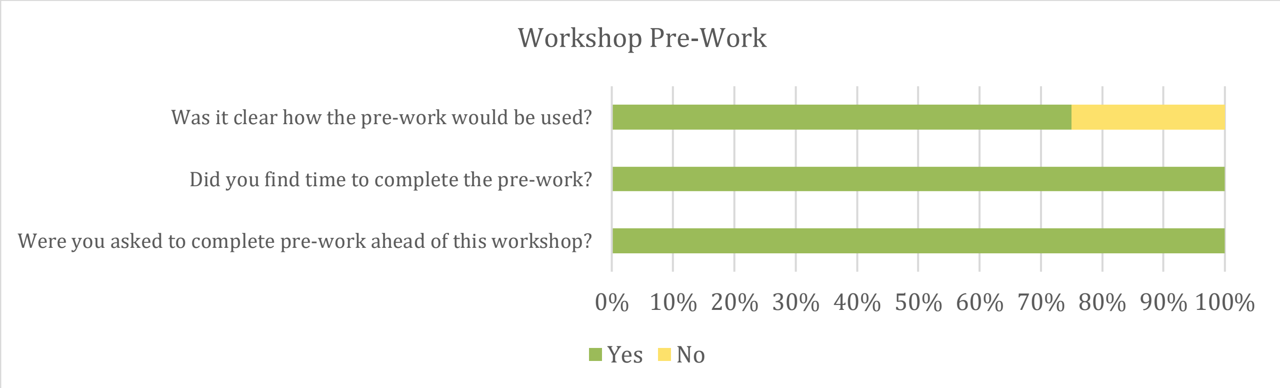
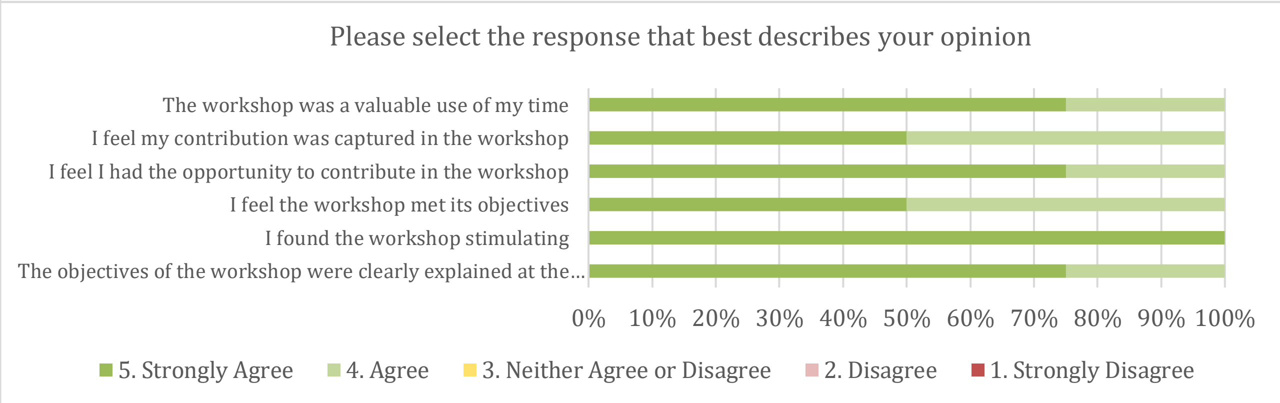
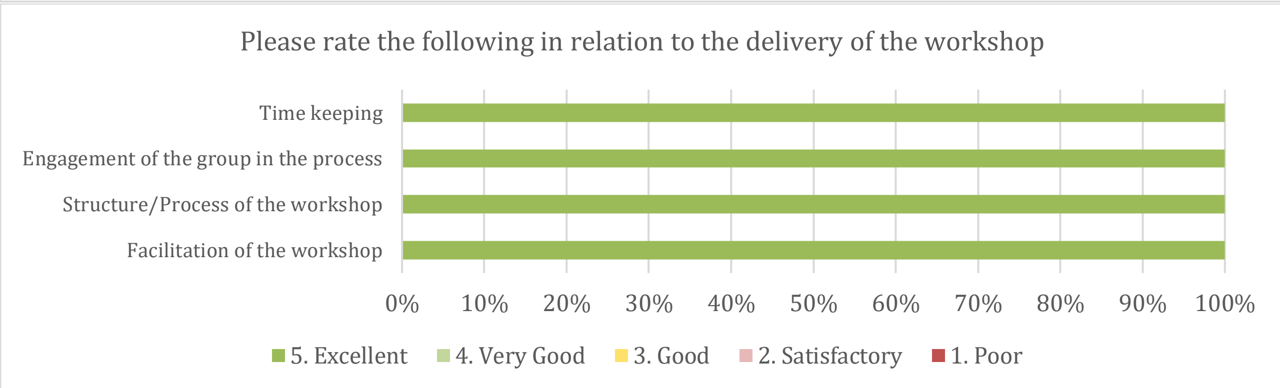
APPENDIX II: PARTICIPANT FEEDBACK

Feedback was received at the end of the workshop from four participants. All of the participants considered the workshop to be Excellent, Very Good or Good, as well as useful and stimulating. All participants considered their participation to be worthwhile and their participation in the workshop a valuable use of their time. The detailed feedback is shown below.







APPENDIX III: WORKSHOP METHODOLOGY

The roadmapping workshop methodology consisted of three parts: design, the workshops, and reporting of the workshop outcomes.

DESIGN

During the design phase, the following activities took place:

- Discussing and designing in detail the workshop methodology and process. The workshop used the **S-Plan** framework developed by the IfM over a period of several years. [148, 149, 150] The framework has been configured to help universities and research organisations align their research activities with industry needs, supporting decision-making and action;
- Designing the templates necessary to support the workshop activities;
- Agreeing the detailed workshop agenda;
- Agreeing the desired workshop outputs.

WORKSHOPS

The roadmapping workshop process brought together 55 participants from the research community and industry and had the following structure:

- First session on 20 March 2020 10:00 – 12:00
    - To **review** the content submitted so far on:
        - Current hydrogen production technologies (scalable to TW level and with the potential to improve efficiencies)
        - Other viable hydrogen generation options available
        - Alternative chemical carriers for hydrogen
        - Required enabling technologies
        - Carbon capture
    - Identify and fill in any **gaps**
    - Review and feedback.

- Second session on 27 March 2020 09:00 – 10:00
    - To **discuss** the results of voting
    - To **select** the priority ideas for the short, medium and long-terms
    - To set up the **working groups** that would explore each idea in Workshop 3

[148] http://www3.eng.cam.ac.uk/research_db/publications/rp108
[149] Phaal, R., *et al.,* 'Customizing Roadmapping', Research Technology Management, 47 (2), 2004, Pages 26–37. https://doi.org/10.1080/08956308.2004.11671616
[150] Phaal, R., *et al.,* 'Strategic Roadmapping: A workshop-based approach for identifying and exploring innovation issues and opportunities', Engineering Management Journal, 19 (1), 2007, Pages 16–24 https://doi.org/10.1080/10429247.2007.11431716

- Third Session on 27 March 2020, 13:00 – 15:00
    - To **explore** selected **key priority** materials for low-carbon hydrogen production
    - To **scope** each priority idea
    - To map **the research and development path** and the required resources
    - To describe **the expected deployment** and the required technological and commercial enablers

- Fourth session on 01 May 2020, 14:00 – 16:00
    - To **explore** how to improve hydroxide conducting polymeric membranes
    - To **scope** the topic
    - To map **the research and development path** and required resources
    - To describe **the expected deployment** and required technological and commercial enablers

- Fifth Session on 05 May 2020, 14:00 – 16:00
    - To **explore** how to develop new conducting and stable materials for PEMWE current collectors, porous transport layers and catalyst support
    - To **scope** the topic
    - To map **the research and development path** and the required resources
    - To describe **the expected deployment** and the required technological and commercial enablers

- Sixth session on 14 May 2020, 14:00 – 16:00
    - To **explore** how to develop improved materials for high temperature electrolytic production of hydrogen and other valuable chemicals
    - To **scope** the topic
    - To map **the research and development path** and the required resources
    - To describe **the expected deployment** and the required technological and commercial enablers

REPORTING OF OUTCOMES

Finally, the IfM ECS transcribed all of the output from the workshop in electronic format, drafted the current report and distributed it to Royce for review and wider circulation.

APPENDIX IV: WORKSHOP AGENDAS

Session 1	
10:00 – 10:05	Welcome from Henry Royce Institute
10:05 – 10:15	Introductions, objectives and workshop 1 process
10:20 – 10:30	Discussing the content collected so far (data provenance and review process)
10:30 – 11:30	Review pre-work and identify gaps for materials and systems (in small groups)
11:30 – 11:55	Feedback review of group review (5 minutes of presentation)
11:55 – 12:00	Wrap-up and process feedback

Session 2	
09:00 – 09:10	Introductions, objectives and workshop 2 process
09:10 – 09:25	Review the short, medium and long-term prioritisation results in groups
09:25 – 09:35	Feedback of review discussion (5 minutes presentation)
09:35 – 09:55	Set up the working groups for exploring the different topics
09:55 – 10:00	Wrap-up and process feedback

Sessions 3, 4, 5 and 6	
13:00 – 13:10	Introductions, objectives and workshop 3process
13:10 – 14:25	Exploration of selected topics
14:25 – 14:55	Presentation and review
14:55 – 15:00	Wrap-up and feedback

APPENDIX V: DETAILED CURRENT AND FUTURE CHALLENGES

	Challenges	Timescale
C1	Public perception and education	ST
C2	Hydrogen is not naturally occurring and takes a large amount of energy to release. A critical issue is where the electricity to undertake electrolysis would originate from.	ST-MT
C3	Hydrogen is difficult to store and distribute.	ST-MT
C4	There is a need for grid scale storage topics, and an integrated energy network linking electricity generation, storage, hydrogen production and storage. Therefore, significant materials innovation and systems integration are required.	ST-MT
C5	The main production technologies that have produced reasonable volumes of compressed hydrogen are not practically scalable, and thus it is essential that alternatives are found.	ST-LT
C6	Industrial sector (reforming, ammonia, minerals, etc.).	ST-MT
C7	Carbon-Neutral Aviation Fuel	LT
C8	Viable technologies	ST-MT
C09	Decarbonisation of chemical production, all industrial-processes (including imported goods) in the UK and establishing low-carbon hydrogen infrastructure from source to delivery point.	ST-MT
C10	Development of Carrier Distribution Network	MT
C11	Subsidies to ensure competitiveness	ST
C12	UK wide H_2 delivery network at appropriate H_2 purity for maximum impact	ST-MT
C13	Policy and regulation for hydrogen economy	ST-MT
C14	Needs to be competitive in relation to the oil and gas industry	ST-MT
C15	Tax on fossil fuels	ST-MT
C16	Understanding of legislation around renewables	ST-MT

APPENDIX VI: DETAILED SOLUTION SCORING

	Low-carbon Methods of Hydrogen Generation	Reward votes	Feasibility votes	Timeline
	A. Low-Temperature Water Electrolysis			
HA1	Develop proton-conducting membranes that are impermeable to H_2 and O_2, which have high conductivity, high strength, high durability and ideally also, are cheaper than the current state-of-the-art, based on Nafion. The development approach needs to be specified, for example, avoiding molecular cross-over; integrate materials; spray approach (Manchester concept); water management; 2D materials. It needs to be operational at higher temperatures to facilitate increased efficiency.	3	3	MT
HA2	Develop hydroxide-conducting membranes that have equivalent conductivity, CO_2 tolerance and stability to the current state-of-the-art proton conducting membrane, Nafion (CO_2 from air poisons alkaline membrane electrolysers). The operating parameters will need to be defined more tightly (e.g. stability, conductivity, gas impermeability, mechanical robustness).	9	7	LT
HA3	Discover anode catalysts that function at pH 0 with 10 to 50 fold lower iridium content than the current state-of-the-art without compromising stability and minimising overpotential. Material recovery, recycling and circular thinking should also be considered.	9	4	MT
HA4	Discover anode catalysts that function at pH 0 without precious metals, with the same performance or better than the current state-of-the-art based on iridium.	8	8	LT
HA5	Discover anode catalysts that function in alkaline media, which minimise overpotential, without compromising stability.	6	2	LT
HA6	Establish stability of Pt catalysts in acid at PEMWE at ultralow loading. Note that the amount of Pt required to drive hydrogen evolution in acid at PEMWEs cathodes is negligible, due to its exceptionally high activity. Hence, the Pt does not pose a barrier to scaling up technology to TW level: research should therefore not be directed towards the discovery of non-precious hydrogen evolution catalysts: The scalability of Ir is several orders of magnitude worse (see Bernt, Gasteiger *et al*. J. Electrochem Soc 2018).	6	4	ST
HA7	Currently in PEMWEs, the cost of the bimetallic plates and porous transport at the anode can exceed the catalyst, as it is challenging to find conducting materials that do not passivate. As such, precious metals are often used to minimise the resistance of titanium components. Moreover, the lack of a stable and conducting support to disperse the catalyst means that high Ir loadings are needed to ensure that the catalyst is not electrically isolated. The discovery of durable materials and precious metal free materials for the transport layer, bimetallic plate and catalyst support would significantly decrease the cost of PEMWEs. There could be plenty of translational impact by adopting processing methods from other areas of materials science (e.g. metallurgy, corrosion science, etc). The coating and material of current collectors corrosion mitigation is also very important. [151]	7	5	MT
HA8	In order to lower the local bubble formation at the catalyst surface, design electrode/porous transport/catalyst layers in anode of electrolyser with a balance between hydrophobicity and hydrophilicity. The focus should be on a technological solution on high current operations.	6	2	MT
HA9	Scalability of production.	1	2	MT
HA10	Community database and sharing best practices to increase performance. Standardisation for testing new catalytic materials and their performance.	10	8	ST
HA11	The study of fouling mechanisms by impurities in water and the development of remediation mechanisms and low-grade water-tolerant catalyst, membranes and electrolyser designs	2	2	MT
	B. High-Temperature Electrolysis and Related Systems			

[151] Bertuccioli, C., David, Lehner, Madden & Standen. 'Development of Water Electrolysis in the European Union. Fuel Cells and hydrogen joint undertaking' https://www.nrel.gov/docs/fy19osti/72740.pdf

HB12	Solid oxide electrolysis producing hydrogen from steam typically works at 100% electrical to chemical efficiency at module level in commercial systems such as Haldor Topsoe or Sunfire. This equates to autothermal mode and has distinct advantages in terms of durability as it avoids thermal stress. Other modes have interest but greater durability challenges. Running at lower current can capture heat energy from waste sources and so delivers higher nominal efficiency or running at higher current than autothermal allows higher production per unit area. High temperature improves kinetics and efficiency, but may limit durability. Recognised materials challenges are: 1. Achieving higher oxygen flux in the air electrode, via good mixed conduction capability, reducing the tendency to delamination at high currents. 2. Avoiding Ni coarsening in conventional SOE cathodes. 3. Minimising electrochemical losses at electrodes through improved electrode compositions to enhance output per unit area of cell, and lowers the overpotential to enhance durability. 4. Improved metallic interconnects or supports to deliver durability. 5. Interface engineering to optimise durability and performance.	5	3	MT
HB13	Integration of SOEC with fuel cells or (SOFC) and/or energy conversion devices, such as gas turbines affords highly efficient large-scale systems.	3	2	ST
HB14	Reduce reliance on critical elements such as cobalt and lanthanides to improve sustainability/cost.	2		MT
HB15	Develop small-scale systems for local generation of hydrogen from PV or wind.	7	7	ST
HB16	Design and manufacture of scalable SOEC systems capable of GW conversion of renewables.	4	1	ST
HB17	Solid proton-conducting oxide electrolysis has potential for lower temperature production of dry hydrogen and especially in process integration.	3	2	MT
HB18	Co-electrolysis of steam and CO2 provides syngas for chemical feedstock production and methanol or kerosene as transport fuels. Oxygen co-product from steam electrolysis offers benefit through integration with other processes.	4	2	MT
HB19	High-pressure operation to improve efficiency and initiate pressurisation of the resultant gas. Develop new materials-mechanical properties key.	6	1	ST
	C. CO_2 Utilisation			
HC20	Electrochemical reduction using better electrode and catalytic materials. Methanol Synthesis/Conversion reactions. Stability for molecule catalysts, selectivity and limited materials are major challenges. Stability and efficiency are issues for inorganic catalyst – requiring both characteristics in catalysis is a major challenge. The reduction products need to be identified. Electrochemical reduction using better electrodes and catalytic materials. A range of molecules can be produced from CO_2 but selectivity is a challenge for many, and long-term catalyst stability is largely unexplored. Fundamental understanding is missing or very recently developed in many cases.	9	5	LT
HC21	Combining electrolysis with anaerobic digestion, producing methane from the CO_2 fraction might get close. This approach is also relevant to other molecules.			MT
HC22	The major effort would be in coupling this process with renewable energy systems – thus, if this is "carbon-free" then the need to get lower temperatures, pressures is less important.	3	2	MT
HC23	CO_2 utilisation may play a role in l-c-h production, but, in the long-term switching approaches to avoid CO_2 generation is essential.	1		LT
HC24	Need to develop CO_2 utilisation technology to re-use the captured CO_2 from steam-reforming of natural gas for H_2 production. What can be done industrially in five years for minimising greenhouse gas emissions is only CCUS. There is no shortage of CO_2 at the moment, and it is likely that there will be significant stores in the future. There is an important public perception piece here – what will be acceptable for people in the future?	3	2	LT
	D. CO_2 Storage			

HD25	We need to find a way in the short to medium-term to store CO_2. The cost of CO_2 capture is high. It is unclear if there is a life-time and stability issue regarding CO_2 capture materials. The environmental impact has also not been assessed.			MT
HD26	Carbon capture in metal oxides. There may be issues of limited capacity.	1		MT
HD27	Reliable methods for monitoring CO_2 and accountability.			ST
	E. Direct Photodriven Processes			
HE28	Photocatalytic hydrogen synthesis through photoreforming of renewable/waste substrates, such as oxygenates, needs to be explored. Such substrates are easier to oxidise than water, with the potential for higher-value oxidation products (e.g. alcohols to aldehydes).	4	2	LT
HE29	Biological and biohybrid approaches to producing hydrogen, employing for example algae or bacteria, coupled with light absorbers/(photo)electrodes, is a developing area of interest.			LT
HE30	Direct photoelectrochemical/photocatalytic water splitting is attracting extensive attention, with 100 m^2 photocatalytic demonstration plants already operational in Japan. Cost projections suggest that, with improved efficiency, some technologies could be cheaper than PV and electrolysis.	6	4	LT
HE31	There is also interest in photodriven reduction of CO_2 and N_2 to yield transportable fuels (e.g. methanol or ammonia) or chemicals (e.g. polymers or chemical feedstocks).	2		LT
HE32	For direct photodriven processes (HC2-HC31), benchmarking should be made against PV + electrolysis. Key challenges are the demonstration of solar to chemical conversion efficiencies > 10%, material durability, stability and lifetime over long-term operation, low-cost materials and operation and continuous-flow catalytic processes. As for all solar-driven processes, the low irradiation density of sunlight requires large area systems, and therefore low-cost materials. Solar concentration may be helpful in some applications. The intermittent nature of sunlight is a further challenge. Photodriven systems may be particularly suited to distributed H_2 generation.	1		LT
	F. Hydrogen derived from bio-waste and renewable sources			ST
HF33	Structured catalysts combining microscopic design of catalysts structures (e.g. encapsulation of cheap transition metals) and macroscopic design of support (e.g. optimisation of open-cell area-to-volume ratios) for steam-reforming of bio-waste and/or bio-chemicals for H_2 production. The catalyst design can tune the intrinsic properties of the active sites, addressing the issues of metal sintering and coke deposition, while the use of structured supports can mitigate the effect raised by transport phenomena on the apparent activity of the catalysts.	2	1	MT
HF34	More work needs to be complete on catalysis in the context of biomass and waste gasification; we might temporarily also include plastic waste leftover recycling to syn-gas, as long as the plastics problem remains. This is potentially a high-cost and energy intensive process, with many processing steps required. It also uses natural gas, although plasma gasification using renewable electricity may be a possibility. It is not clear what happens to the CO_2 produced.			MT
HF35	Any use of natural gas increases GHG emissions (even if temporarily stored away). The use of biogas or syn-gas from biomass gasification is the only way to reduce GHG emissions - there is no need to further improve processes, although this will always help. Upscaling biogas and syngas via for example Fischer-Tropsch to suitable fuels (for instance in the hard to decarbonise aviation sector) makes the most sense in the use of this source.			MT
HF36	Instead of hydrogen from bio-resources, it is more useful to use bio-resources for fuels, because of the difficulty to in decarbonising some parts of the transport sector (aviation for example)	2		ST
	G. Steam Reforming			ST

HG37	Improve process and heat integration of current plants through improved reactor design. Utilising membranes and membrane reactors: selective hydrogen separation at intermediate temperature (400-600 °C) using palladium-based membrane has been developed in the recent years. The combination of reaction and separation can shift the current equilibrium conversion toward the products. The hydrogen recovery efficiency can therefore reach above 90%.	1		ST
HG38	The current process of methane steam reforming to produce hydrogen can meet the requirements of TW, depending on how much hydrogen is needed to produce in factory. High-temperature alloy materials for very large reactors may be the key. At present, the atomic chemical reaction efficiency and plant scale of hydrogen production process from fossil energy are very high. If we want to continue to improve the conversion efficiency to go beyond the ~80%, so we must achieve a significant breakthrough in the fundamental research of reaction path mechanism, catalyst and catalytic carrier material. The use of gas-solid reactions with transient metal oxides (Fe, Cu, Ni, Mn or combination a of), as well as the use of high and intermediate temperature adsorption materials, can lead to an increase in overall efficiencies (+5 to 10% higher) of the hydrogen production efficiency by reducing the energy cost. This is particularly true when combined with CO_2 capture since the cost of CO_2 separation is very limited (CO_2 avoidance cost is 20-30% lower than state-of-the-art technology based on solvents). This technology is able to achieve 95% of CO_2 capture. The technologies are suitable to operate several feedstock, including existing gaseous and liquid fossil fuels or derived, bio-based feedstock or waste gas already available in industrial settings such as chemical plant, steelwork. The technology is modular and therefore applicable at different size. Synergies can be achieved via system/thermal integration, combining Exo and Endo - thermic systems. high and intermediate temperature materials need to be developed for *in-situ* carbon capture	2	1	MT
HG39	Integration of steam methane reforming with high-temperature fuel cells increases the overall efficiency of the process, as heat needed for the reforming is provided from the fuel cell operation, and little or no gas combustion is needed. Materials for selective recycle devices are needed to optimise this process. These are mild electrolyser devices operating between fuel streams of varying oxidant content (see the patents of M Bozzolo, device 38 in patent US9972855B2). Counter-intuitively reducing the temperature provides no benefit as corrosion in the support materials increases as the temperature is lowered and the steam methane reforming will deliver lower yields. The oxygen electrode needs to be able to produce a lot of oxygen; the hydrogen electrode needs to be durable – these are key developments.			MT
HG40	Partial oxidation or other conventional processes for handling heavier hydrocarbons.	1	1	ST
HG41	Pyrolysis of methane can yield solid carbon and hydrogen. Some technologies driven by electrical energy have already been scaled up.	1		ST
HG42	100% carbon capture from SMR/ATR.	2	2	ST
	H. Integrated Systems			ST
HH43	Work on the efficiency of an integrated system that started from feedstock and went right through to the user. It must include all manufacturing steps, distribution steps and use steps. It must also include the cost of carbon capture and storage if this is being used. There is no definitive research on the efficiency of an integrated hydrogen system in activities other than industrial settings. Materials that could improve the integrated system are really worth investigating with a rigorous scientific approach.	2		MT

HH44	The main alternative to current production technologies would be a permeation/electrolysis-based system. To achieve efficiency this would need to be a device operating at elevated temperatures (several hundred degrees Celsius). This is likely to preclude polymer-based devices and is likely to direct attention towards ceramics. A critical issue is where the electricity to undertake electrolysis would originate from. Presumably excess capacity from renewable generation would be stored, hence the need for grid scale storage topics, and an integrated energy network linking electricity generation, storage, hydrogen production and storage would be required. Therefore, significant materials innovation and systems integration are required. This depends on how efficiency is defined. With steam methane reforming at 800 °C then there is a thermal efficiency of ~80%. To achieve higher efficiencies, it is likely that processes such as high temperature steam electrolysis or thermochemical water splitting will be utilised, but this will require new materials with catalytic properties and durability. This will mean that materials have to operate in an optimised temperature window, and as such proton conducting oxide ceramics are extremely attractive. To utilise the technology these will have to be coupled with catalysts for oxygen and hydrogen evolution, for example depending on the mode of operation. Effective low-cost catalysts are a significant challenge.			MT
HH45	Carbon capture is unlikely, except in the case of using methane in a syngas production process based on permeation across a ceramic membrane. Here, the CH_4 combines with O_2 from the membrane to produce a CO/H_2 mixture. This can then be kept is a closed cycle, with CO producing CO_2, and this is possibly used in a co-electrolysis cell (CO_2/H_2O). Combining carbon capture with thermochemical utilisation using hydrogen.	2		ST
HH46	Develop durable electrode and electrolyte materials capable of intermediate temperature operation.			MT
	I. Hydrogen Storage and Hydrogen Carriers			ST
HI47	Hydrogen storage and distribution costs are extremely high and this is another area where research is required. Not only is the storage technology (high pressure gas tanks) poor, but the measurement and flow rates around how much hydrogen there is and where it is are also challenging. Materials challenges include: high-pressure tank materials, materials-based storage for mobile applications, metal hydrides for stationary storage with initial hydrogen compression, and materials for hydrogen sensing applications.	1		MT
HI48	It is also important to think about sustainable synthesis of chemical feedstocks using H_2 or directly through power to chemicals. Materials challenges include: new materials for solid oxide-based electrolysis for chemicals manufacture, catalysts for efficient conversion processes.	3	1	MT
HI49	The reversible reaction from toluene to methyl-cyclohexane, and back is another hydrogen carrier. The advantage is that these are benign materials that are readily available and can be safely recycled. It has also been investigated by Hrein in Japan and proven at small scale. The problematic step is the endothermic process to extract the hydrogen from the methyl-cyclohexane in low-volume dispersed application. Materials challenges include: catalyst design and carrier modification to improve kinetics.	1	1	LT
HI50	Ammonia is an excellent carbon-free hydrogen carrier or energy vector because it does not have storage problem and has mature large-scale synthesis (Haber-Bosch) and distribution systems. There is a need to develop materials for small-scale and intermittent ammonia synthesis and for converting the chemical energy in ammonia into electricity (fuel cells, combustion, gas turbines). Materials challenges include: electrocatalysts for ammonia production and decomposition, catalysts for low-temperature conversion of ammonia to hydrogen and nitrogen, direct ammonia fuel cells, ammonia absorption materials for integration into HB synthesis to improve yield and efficiency , improved NOx reduction materials, and improved alloys for membrane purification of ammonia-derived hydrogen (high temp and low temp).	5	3	MT

HI51	Multifunctional materials in hydrogen systems, for example, whole-system hydrogen storage from electrolyser to fuel cell without compressors and dehumidifiers/humidifiers. Materials challenges include: design of materials with tailored/flexible hydrogen storage and release properties that can be integrated with hydrogen production/use and reduce the need for compressors. Integration of metal hydrides into regenerative fuel cell systems.	4	1	LT
HI52	Examination of the materials properties of the existing gas grid for suitability for high % levels of hydrogen. Materials challenges include: hydrogen leakage/safety, long-term durability.	6	3	ST
HI53	A key challenge for getting to the TW scale is developing routes for international transport of large amounts of stored renewable energy from low-cost electricity regions in the form of chemical fuels synthesised sustainably, e.g. H_2, CH_4, methanol and ammonia. Materials challenges include: materials for fuel synthesis and decomposition (catalysts, electrochemical devices), and materials considerations for integrated electrolysis and conversion systems.	9	5	LT
	J. Other			ST
HJ54	Deconstruction of hydrogen production materials to simple components that can be reassembled into catalysts. System approach to design step, rather than the current practice of thinking about it at the end.	1		ST
HJ55	Heat storage in metal-organic frameworks.			LT
HJ56	Thermocatalytic methane pyrolysis – trying to convert CH_4 to a higher value carbon product – hydrogen is currently a by-product.	1		LT
HJ57	Plasma decomposition of methane – interesting projects already.	1	1	ST
HJ58	Thermochemical water splitting – requires high temperatures. Metal oxide cycling. Research currently in this area.	2	1	LT
HJ59	Purity and purification, could be electrochemical. Catalyst could be destroyed with impurities.	5		ST
HJ60	Selective separation of Hydrogen with natural gas	1	1	ST

Figure 13: Detailed scoring of proposed low carbon methods of hydrogen generation

APPENDIX VII: DETAILED RESEARCH, TECHNOLOGY, ENABLERS

	Research, Technology, Enablers	Timescale
R1	Simulation tools to discover new materials *in silico*. This is key to accelerating material discovery.	ST-MT
R2	Analytical techniques for driving real understanding of the conversion processes, and allows us to "see" what's going on in real time. Generating understanding of processes for optimisation.	ST-MT
R3	Identification of active catalyst state.	State-of-the-art
R4	Hybrid water-splitting techniques and chemical looping.	ST-MT
R5	Humidity capture for heat storage in hydrogen tank.	ST
R6	Efficient reactor designs for various chemistries.	MT
R7	Electrochemical hydrogen compression technologies .	MT
R8	Fundamental surface science of e.g. electrolysis, catalysis, steam reforming, etc. the processes that make hydrogen.	ST-MT
R9	Hydrogen-on-demand fuel tanks + fuel cell engines.	MT-LT
R10	Phase control for metallic TMD catalysts.	ST-MT
R11	Better understanding of reaction mechanisms.	MT
R12	More efficient microbial systems for higher Cn compounds.	MT-LT
R13	Reduced or even non-precious metal content catalyst layers for PEMWE.	MT-LT
R14	Durable and active AEM membrane development.	MT-LT
R15	Wind power, hydroelectric, solar cells, etc. (renewables).	ST
R16	Professional, independent facilities for short- and long-term operando testing (including synchrotron facilities and neutron imaging) and validation of new materials under the relevant conditions. Imaging of catalyst layers *in-situ* and *ex-situ* testing.	ST-LT
R17	High throughput testing for new and novel catalyst motifs, including engaging with computational chemists.	MT
R18	Partnerships: an interaction between academic and industrial partners who understand how things will operate in a stack and what the real need is, academia who can develop new materials and methods and research institutes who can bridge the gap and support scale-up and testing. e.g. Horizon 2020 projects in the UK.	ST-LT
R19	Facilities for *in-operando* testing of catalysts.	MT-LT
R20	High throughput testing for catalysts Imaging of catalyst layers *in-situ* and *ex-situ* testing (already done in fuel cells).	ST-LT

R21	Access to synchrotron facilities and neutron imaging.	ST
R22	Table-top synchrotrons (groups in Korea and China working on these).	MT-LT
R23	Moving towards single atom catalysts to reduce the amount of Pt and Iridium catalysts used.	MT
R24	Device and system design and manufacturing.	MT-LT
R25	Experimental materials discovery assisted by computation.	ST-LT

APPENDIX VIII: LIST OF FIGURES

APPENDIX VIX: LIST OF TABLES