MATERIALS FOR END-TO-END HYDROGEN

This report is commissioned by the Henry Royce Institute for advanced materials as part of its role around convening and supporting the UK advanced materials community to help promote and develop new research activity.

The overriding objective is to bring together the advanced materials community to discuss, analyse and assimilate opportunities for emerging materials research for economic and societal benefit. Such research is ultimately linked to both national and global drivers, namely Transition to Zero Carbon, Sustainable Manufacture, Digital & Communications, Circular Economy as well as Health & Wellbeing.

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Materials for end-to-end hydrogen

An overview of materials research challenges to be addressed to facilitate increased uptake of hydrogen in energy applications

Final report

April 2021

Commissioned by the Henry Royce Institute

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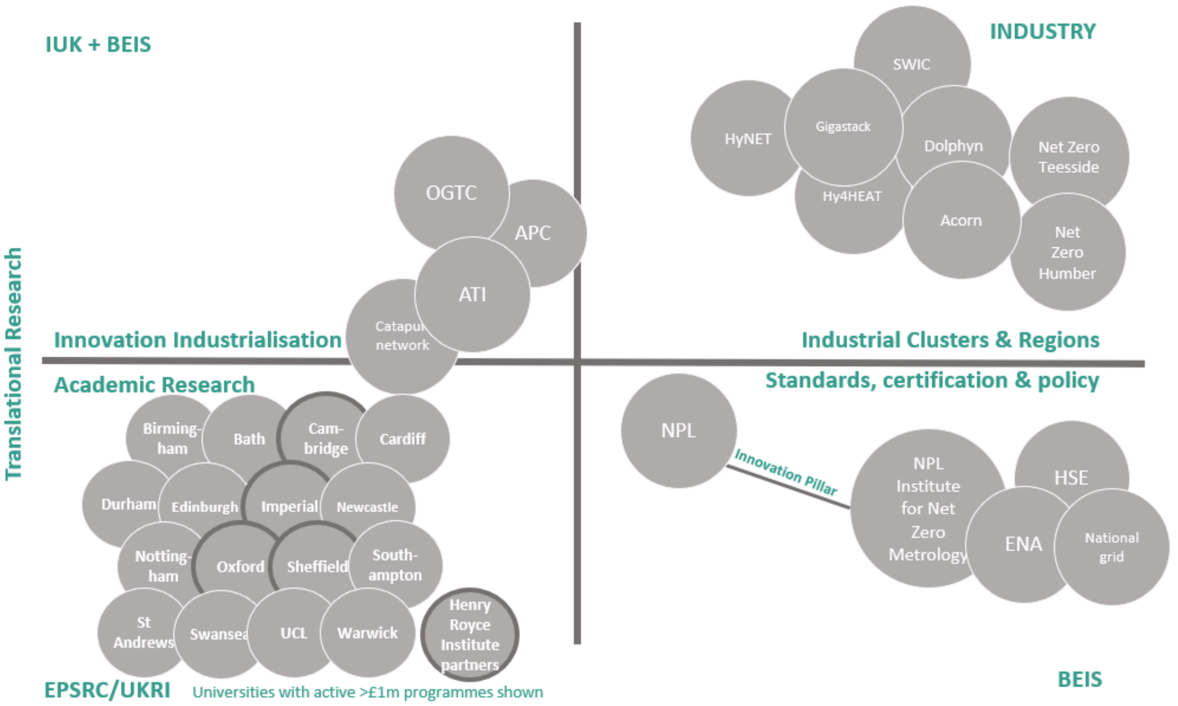
Foreword

The Henry Royce Institute has led an exercise to elicit the views of a wide range of stakeholders, from academia and industry, on the principal materials research challenges to be addressed to enable hydrogen use in energy applications. The study comes at a time when the hydrogen sector is on the cusp of significant growth.

Embarking on this study, it is important to acknowledge the significant body of work that preceded it and the work that continues today (the figure below provides an illustration of major current UK activities). A collaborative approach was adopted from the outset, to ensure this study would build on preceding activity and reflect the views of the industry and academic community that provided input.

Illustration of UK projects supported in the hydrogen space



Key

APC – Advanced Propulsion Centre UK
ATI – Aerospace Technology Institute
BEIS – Department of Business, Energy, and Industrial Strategy
ENA – Energy Networks Association
EPSRC - Engineering and Physical Sciences Research Council
HSE – Health and Safety Executive
IUK – Innovate UK
NPL – National Physical Laboratory
OGTC – Oil & Gas Technology Centre
SWIC – South Wales Industrial Cluster

This report outlines the key materials research challenges to enable hydrogen to be produced, stored and distributed at scale, to decarbonise a range of sectors in a 2050 timescale. The objective is to identify the five materials areas critical to enabling the widespread use of low-carbon hydrogen in a UK context, while maintaining a perspective of opportunities in global deployment. The selection criteria that were employed to identify these areas are based on impact, timing, and the UK's potential to lead. The driver behind criteria selection is to ensure further investment in skills and resources, focused on areas where the benefits accrue to the UK. The report also identified a range of other technology areas beyond the five key materials areas. These innovations require further detailed review, to identify potential for future disruptive solutions.

This report comes at a time when significant levels of investment are being targeted on the global scaling up of the generation and use of hydrogen derived from low carbon and renewable energy sources. The findings reported here illustrate the fundamental role that materials can play in delivering this growth, and they highlight the UK opportunities to take leadership positions in critical areas of this fast-developing sector.

Following this report, the next phase of this work will identify the resources and partnerships required to realise the UK's leadership ambitions in these key materials fields. This will help to enable the potential wider role for hydrogen to be used as an energy vector in delivering net-zero targets with a 2050 timescale.

Dr Robert Michael Sorrell – Hydrogen Challenge Lead, Robin Morris – Business Development Lead, Henry Royce Institute

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Executive Summary

The global hydrogen energy sector is on the cusp of rapid growth, with hundreds of billions of dollars of investment being committed by governments and industry to develop systems for renewable and low carbon hydrogen production and end-use [1]. There is currently a focus on deployment of first-generation technology solutions at scale, to meet short and medium-term targets. An example of this is the ambition to install 6GW of electrolysis by 2024 and 40GW by 2030, as set out in the EU Hydrogen Strategy [2]. There is significant scope for further research and development to deliver cost and performance gains across the hydrogen value chain, as required for wider scale deployment. Addressing fundamental materials science issues will be an important enabler for further roll-out of hydrogen in energy applications, and this is a space in which the UK benefits from world-leading expertise.

In this study, the Henry Royce Institute led an exercise to elicit the views of a wide range of stakeholders from academia and industry on the principal materials research challenges to be addressed to enable increased use of hydrogen in energy applications. The work builds on the *Materials for the Energy Transition* roadmaps published in 2020 [3], one of which focused on low carbon production of hydrogen and related energy carriers. This paper expands the scope, by considering the entire hydrogen value chain: production, storage, distribution, and use. Expert representatives from the research and industry communities were consulted through a series of bilateral discussions, questionnaires, and workshops carried out during the first quarter of 2021.

The report summarises the materials technology areas recognised as having the potential to provide a significant contribution to realising hydrogen deployment at scale. These technologies vary substantially in their level of technical maturity and risk. The study identifies and prioritises the five key materials areas core to enabling hydrogen's role in delivering the UK's 2050 net zero targets. Their identification is based on a combination of industry and academic input; and a set of criteria around timing, impact and UK leadership capabilities. The objective is to identify the technology areas that will make the most significant impact in a 2050 timescale and in which the UK has the capability to lead. The report identifies several technologies beyond the five critical technology areas. The aim is to encourage further detailed review of these to identify any potential future game-changers. The five key materials research areas that have been identified are:

- **Reducing iridium loading in polymer electrolyte membrane (PEM) electrolysers to realise global electrolysis capacity ambitions at a terawatt (TW) scale.** The UK is well placed to exploit its expertise in catalysts, nanoengineering, and PEM electrolysis, to become a world leader in this area.
- **Improving catalysts for distributed ammonia production and cracking, to realise ammonia's potential as a hydrogen storage and distribution vector**. The UK is well positioned to lead in this field with expertise in catalysis and nanoengineering.
- **Improving point of use hydrogen purification technologies, enabling large scale fuel cell hydrogen supply from the gas grid**. The UK has expertise in technologies for hydrogen deblending from the gas grid, such as membranes and pressure swing adsorption.
- **Detailed understanding of materials degradation pathways for high volume compressors to enable large scale hydrogen distribution through the UK gas grid.** A number of major UK projects are currently reliant on this approach being effective at scale.
- **Materials led solutions for cost effective, conformable hydrogen tank storage in fuel cell vehicles**. The UK has significant experience and knowledge of composite materials relevant for addressing this challenge.

The study's findings inform the immediate direction for UK materials research in hydrogen energy applications. Addressing these materials challenges will support the UK's wider leadership ambitions in the hydrogen energy sector, by offering potential materials solutions to accelerate hydrogen deployment. A key objective in presenting this report is to catalyse further investment and collaboration between academia and industrial organisations, to facilitate research and innovation to enable development of appropriate solutions in this space.

Contents

1. Introduction

Global context

Governments have accepted the need to completely remove greenhouse gas emissions from the energy system to meet the challenge of climate change, with 196 parties signing the Paris Agreement in 2016, to limit global warming to well below 2°C [4]. A full suite of all available options are required to address this challenge. Hydrogen offers promise as an energy vector that can be produced from a range of sources, facilitating increased harnessing of renewables, and providing long-term energy storage at scale. This will enable decarbonisation of several hard-to-abate areas across the power, heat, and transport sectors. Although not a silver bullet for the energy and environmental challenges faced, hydrogen is becoming a key element in strategies to achieve net zero carbon emissions by public and private sector stakeholders around the world.

The Hydrogen Council, an international CEO initiative seeking to foster the role of hydrogen in the energy transition, now comprises over 100 global companies [5]. It has published a vision for how hydrogen can simultaneously support the deployment of additional renewable power sources, such as wind or solar power, and decarbonising activities in multiple "hard to treat" sectors [6]. National hydrogen strategies have been published in recent years by countries around the world (including Germany, France, Spain, Portugal, the Netherlands, Norway, Japan, South Korea, and Australia), and hydrogen strategies are being prepared by many others, including the UK.

The European Hydrogen Strategy, published in July 2020, sets a target to install a minimum of 40GW of electrolysis capacity in Europe by 2030. It envisages hydrogen becoming an intrinsic part of the energy system over the coming decades [2]. In November 2020, the UK Government published its Ten Point Plan for a Green Industrial Revolution, which sets a target for the UK to develop 5GW of low carbon hydrogen production capacity by 2030 [7]. The UK Hydrogen Strategy is due to be published by mid-2021.

While the use of hydrogen in energy applications to date has been restricted to relatively niche application areas, the 2020s is set to be a decade in which the hydrogen energy sector develops and matures from both a technical and commercial perspective. The European Hydrogen Strategy states that hydrogen will need to become 'an intrinsic part of our integrated energy system' by 2030 [2].

Study context and objectives

Henry Royce Institute

The Royce Institute is a UK national centre for research and innovation of advanced materials. It operates as a hub and spoke model, with the hub at The University of Manchester, and spokes at the founding partners, initially comprising the universities of Sheffield, Leeds, Liverpool, Cambridge, Oxford, and Imperial College London, as well as UKAEA (Atomic Energy Authority) and National Nuclear Laboratory.

In 2020, the Henry Royce Institute led a UK-wide consultation on Materials for the Energy Transition. In September 2020, the Royce Institute published a set of five roadmaps resulting from this process, including one focused on materials for low carbon production of hydrogen, related energy carriers and chemical feedstocks. This study builds on work completed in the roadmap, by considering the materials research needs to support the entire hydrogen value chain. It is expected that the findings will be used as the basis for the development of the UK's strategy on materials research to support hydrogen technologies.

With hydrogen increasingly becoming an integral component of future energy systems there is an opportunity for the UK to invest in hydrogen technology development. Given the academic and industrial expertise in hydrogen and materials currently existing in the UK, the country is well placed to be at the forefront of this technology development. This expertise has been used to facilitate the identification of the research priorities for new or improved materials to support hydrogen use at scale in the energy sector on a 2050 timescale in this report. Priority was given to areas where the UK has clear expertise or is developing the capability to lead, along with areas which specifically benefit UK hydrogen usage, e.g. enabling the coupling of hydrogen to offshore wind – a plentiful UK resource – or exploiting existing natural gas transmission and distribution networks.

Scope and methodology

A focused approach was adopted, to identify the key materials challenges across the hydrogen value chain; covering hydrogen production, storage and distribution, and end use.

The study team, led by Royce with support from delivery partners (see box), adopted a consultative approach. The findings and recommendations summarised in this report reflect feedback from the community working in this area. The engagement exercise, which took place during the first three months of 2021, involved:

- A series of structured interviews with experts from academia and industry.
- A questionnaire (online survey) publicised through networks such as the UK Hydrogen and Fuel Cell Association (UK HFCA), the Scottish Hydrogen and Fuel Cell Association (SHFCA), H2FC SUPERGEN, and Hydrogen London as well as Royce newsletter and website, and KTN specialist communities.
- A workshop with representatives from the gas network operators.
- A set of workshops involving over 60 representatives from the academic and business communities active in this area facilitated by the KTN. Representatives were selected from over 130 expressions of interest submitted.
- Feedback sessions, to develop and confirm the main findings.

Materials for end-to-end hydrogen: study team

Lead	HENRY ROYCE INSTITUTE
Project Champion	**Robert Sorrell**
Project management & consultancy support	elementenergy
Workshop facilitation and stakeholder engagement	ktn ena energynetworks association
Delivery partner	KNOWLEDGE CENTRE MATERIALS CHEMISTRY

The study team made efforts to consult as widely as possible, to collect a representative range of views and develop a consensus on the key materials developments required to support the hydrogen value chain. The authors are grateful to all stakeholders who contributed to the study and to those who provided feedback on the emerging conclusions.

Report structure

The following sections present the materials research challenges identified in each of the main areas of the hydrogen value chain: production, storage and distribution, and end use, with separate sections on end uses in transport, and heat and power. Each section begins with a brief introduction to provide context[1], followed by a summary of the findings from the study. Section 6 provides an overview of the key enabling research areas to support development of materials for hydrogen, and the conclusions are provided in section 7.

Two appendices are included at the end of the report. Appendix I lists those materials for hydrogen topics that were discussed during the workshops but which were not included within the main body of this report. Appendix II addresses the materials research required to enable hydrogen use as a low carbon feedstock in sustainable chemistry applications. This will be the topic of a future road mapping exercise and is therefore beyond the scope of this report.

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[1] The aim is not to provide a comprehensive description of each element of the hydrogen value chain given the substantial quantity of existing literature relating to the hydrogen sector and the aspiration to provide a concise summary of the study in this report.

2. Hydrogen Production

Introduction

Hydrogen is widely used today in a range of industrial processes, principally ammonia manufacture for fertilizers and oil refining. One of the advantages of hydrogen is the diversity of available production options, including:

- *Thermochemical* – steam methane reformation, partial oxidation / gasification, and autothermal reforming are the principal production methods in use today. The carbon footprint of these methods can be reduced by combining them with carbon capture and storage (commonly referred to as “blue” hydrogen).
- *Electrolytic* – the most mature forms of electrolysers currently available are alkaline and polymer electrolyte membrane (PEM). Other technologies at a lower technology readiness level include anion exchange membrane (AEM) electrolysis and solid oxide electrolysis. Low carbon hydrogen can be produced by powering electrolysers with renewable electricity (often termed “green” hydrogen).
- *Biochemical* – options include anaerobic digestion, and novel methods such as photo-fermentation.

For hydrogen to play a role in the decarbonised energy systems of the future, there is clearly a need to transition from traditional production methods to low carbon and ultimately fully renewable solutions. UK expertise in green hydrogen production currently focuses on PEM electrolysis and solid oxide electrolysers. There is little UK academic or commercial interest in alkaline electrolysers [3], and given that this technology is relatively mature, the opportunity for the UK to ‘catch up’ with research efforts being undertaken elsewhere is limited; alkaline electrolysers are therefore not discussed further here. More information on the materials challenges around alkaline electrolysers can be found in a previous Henry Royce study on the materials needs to support hydrogen production [3].

Anion exchange electrolysers could be highly beneficial to the UK since they feature fast response times and could be integrated with intermittent sources of electricity such as offshore wind. Conversely, solid oxide electrolysers are limited by their high operating temperature, which makes the technology best suited for integration with a constant source of heat and power, such as a high temperature nuclear reactor [8] or solar heat generators and photovoltaics [9].

Key materials research challenges

Key priority: Reducing iridium loading in polymer electrolyte membrane (PEM) electrolysers

PEM electrolysers contain rare and expensive elements to catalyse the process of hydrogen and oxygen evolution at the cathode and anode respectively. These elements increase the capital cost of PEM electrolysers, thereby increasing the cost of green hydrogen. The global production capacity of these rare elements will place limits on the electrolysis capacity that can be developed at current catalyst loading levels. A reduction in rare element loading, particularly iridium, will be required to realise PEM electrolysis capacity on a terawatt scale.

Maximising the efficiency of hydrogen production via electrolysis is important to minimise the costs of green hydrogen, as input energy is a key component of the production cost. PEM electrolysers use catalysts based on rare metals at both the anode and cathode, to minimise the specific energy consumption (kWh/kg) of the stacks. Choice of catalyst is currently limited to the relatively rare and costly platinum group metals due to the harsh conditions in PEM electrolysers – low pH, high potential, and high oxygen concentration [10]. PEM electrolysers, such as those produced by ITM Power, can achieve a specific energy consumption of below 60kWh/kg [11]. In 2018, a European partnership, The Fuel Cells and Hydrogen Joint Undertaking (FCH JU), set a target specific energy consumption for PEM electrolysers of 55 kWh/kg in 2020, improving to 50 kWh/kg by 2030 [12]. New catalysts will therefore need to maintain or improve the efficiency of PEM electrolysis.

The previous Henry Royce report on materials needs for low-carbon hydrogen production [3] estimated the length of time to produce sufficient iridium and platinum to support 1TW of PEM electrolysis capacity. While this is a long-term challenge for PEM electrolysers, which are currently only manufactured in the tens of MW per year [11]; if hydrogen is adopted globally significantly more electrolysis capacity will be required. IRENA estimate that between 4 and 16 TW of wind and solar capacity could be required for hydrogen production alone by 2050 [13].

State-of-the-art PEM electrolysers require 1–3mg/cm^2 of platinum group metals (iridium and ruthenium-based oxides) to catalyse oxygen evolution at the anode [3]. The Henry Royce study on materials for low-carbon hydrogen production estimated that over 27 years of the 9 tonne/year global iridium production would be required to develop 1TW of PEM electrolyser capacity [3], which is clearly a limitation. It is estimated a 40-fold reduction in PEM electrolyser iridium loading is required for large-scale electrolysis [10]. High demand for iridium, long processing times, limited supply, and an undiversified supply chain [14] have already caused the price of the metal to increase nearly four-fold, from $1,670/Oz on 1st December 2020 to $6,000/Oz by the end of March 2021 [15]. Without new materials solutions to reduce iridium loading in PEM electrolysers, volatility in iridium price and lack of availability will impact the viability of large-scale PEM electrolysis.

Platinum is used to catalyse hydrogen evolution at the cathode of PEM electrolysers. The Royce materials for low-carbon hydrogen production report estimates that, with 0.025mg/cm^2 platinum loading, the production of 1TW of PEM electrolysis would require only 0.02 years of the annual 200 tonnes/year global platinum production capacity [3]. Reducing iridium loading is therefore a more urgent research challenge than reducing platinum loading.

Materials research should aim to enable reductions in rare material loading in electrolysers while maintaining (or ideally improving) electrolyser efficiency and durability. Incremental improvements to catalyst performance may be achieved by screening large numbers of catalyst materials (through a combination of computational aided design and physical testing). It is expected that step-changes in catalyst performance will be delivered via deeper understanding of methods to reduce catalyst loading. Nanoengineering will play a key role in turning inactive sites into active sites, thus minimising catalyst loading requirements.

Research to support the reduction of rare material use in electrolysers is not limited to the development of new catalysts. It will need to consider all materials in the overall electrolyser system. For example, it is likely the development of new substrates (such as titanium dioxide-based substrate materials) that are stable in the acidic, oxygen rich environments found in PEM electrolysers, will be required to support single-site catalysis.

Development of new materials should be aligned with an understanding of the economic and lifecycle impact of raw materials on the electrolyser supply chain. This topic is explored in section 6 of this report. Industry collaboration is required to benchmark catalyst properties, and to share data on catalyst performance characteristics, to help focus research efforts on the most promising areas.

Case study: UK expertise on PEM electrolysis

The UK is well placed to work on this challenge, given the expertise in PEM electrolysis from businesses such as ITM Power, one of the world's leading PEM electrolyser manufacturers. ITM Power is in the process of significantly increasing its manufacturing capacity and the size of the electrolyser modules. Further, the UK has specialists across academia and industry in catalysis, from companies such as Johnson Matthey, and expertise from the UK Catalysis Hub, Cardiff Catalyst Institute, and Imperial College. Beyond catalyst expertise, knowledge of nanoengineering is also expected to lead to new insights about catalyst performance, through organisations such as the London Centre for Nanotechnology.

Further materials research challenges

Beyond the key research topic of reducing scarce material loading in PEM electrolysers, the following were considered to have significant potential as materials research areas:

- **Anion exchange membrane electrolysers** are currently at a lower technology readiness level than PEM or alkaline electrolysis. They combine the benefits of both technologies, leading to compact, low-cost electrolysis with no scarce metal loading in the electrodes and the option to generate hydrogen at above-atmospheric pressure (tens of bar).
- **Solid oxide electrolysers** are at a lower technology readiness level than PEM or alkaline electrolysers. They offer the potential for higher electrical efficiency hydrogen production. These electrolysers operate at a high temperature and have slower response times, and are therefore suited to applications where a constant source of high temperature heat and power is available.
- **Marinization of electrolysers** will allow the direct coupling of electrolysers to offshore wind enabling energy to be transported to shore in the form of hydrogen, at a potentially lower cost than transporting electricity.
- **Solar water splitting** is at a very early stage of development but would offer a step change in hydrogen production technology in a field where the UK has materials research experience.

Further information on each of these areas is provided below.

Anion exchange membrane electrolysers

While at a relatively early stage of development compared with alkaline and PEM electrolysis, anion exchange membrane (AEM) electrolysers may, in future, be able to offer advantages over alternatives [16]*. Through the use of a membrane electrolyser in mildly alkaline conditions, AEM electrolysers are able to combine the relative advantages of alkaline (low cost, abundant materials) and PEM technologies (compact design, ability to pressurise hydrogen, pure water feed)* [16] [17]*. Improvements to several materials aspects within the AEM cell are required to improve performance and durability.*

AEM electrolysers have two distinct advantages over PEM electrolysers with regards to the cost of materials used:

- Platinum group metals are not required for the electrodes of AEM electrolysers, thereby reducing cost and mitigating the risk of limited electrolysis capacity being produced due to limited availability of scarce metals.
- While PEM electrolysers require titanium-based bipolar plates to achieve high current densities in an acidic environment, AEM electrolyser can use lower cost stainless steel current collectors [16].

The mildly alkaline conditions of AEM electrolysers allow them to use a pure water feed, as opposed to alkaline electrolysers which require alkaline water feed. These pH conditions lead to materials challenges around reaction kinetics and material stability. The composition and activity of AEM electrocatalysts must be optimised for AEM pH conditions to avoid a reduction in reaction kinetics. The membrane and ionomer are known to have limited thermal stability under these conditions due to the degradation mechanisms that occur under high pH [16]. To improve AEM electrolyser operation, materials developments are required to increase the chemical and thermal stability of the cells [17].

Case study: Development of AEM expertise

AEM expertise is currently being developed across Europe, with Fuel Cells and Hydrogen Joint Undertaking (FCH JU) funded projects. Companies such as Evonik and Enapter are investing in the development of AEM technologies. Since the technology is currently at an early stage, investment in AEM research will enable the UK to develop world-leading capabilities in these electrolysers.

While AEM technology benefits from the use of non-precious metal catalysts, the low activity of these catalysts requires high loadings, resulting in increased resistance and reduced efficiency. The ionic conductivity of the ionomer and membrane requires improvement, potentially through the development of thinner membranes [17].

Improve material stability and lifetime in solid oxide electrolysers

Previous experience indicates that material stability in solid oxide electrolysers is a key issue with accelerated material degradation occurring at the high operating temperatures (500 – 1,000°C). Future solutions require electrolysers to have lower degradation rates than the current 1.9–2.4%/1,000 hours of operation. Current efficiencies of 40–41 kWh/kg of electrical input will be required (FCH 2 JU 2017 state-of-the-art and 2020 target efficiencies [12]*), with a 2030 target of 37 kWh/kg of electrical input set by the FCH JU* [12]*.*

There are typically three key materials that form a solid oxide electrolyser system:

- **Electrolyte**: Yttria-stabilized zirconia (YSZ) which allows diffusion of oxygen but not electrons. The electrolyte has excellent ionic conductivity between 800°C and 1000°C but exhibits reduced ionic conductivity at lower temperatures. Since a decreased operating temperature would improve the durability of materials in solid oxide electrolysers, work is being undertaken to modify YSZ electrolytes to increase ionic conductivity at low (<600°C) temperatures [18].
- **Steam/H_2 electrode**: A ceramic-metal composite material of nickel (Ni-YSZ) is often used; perovskite-type lanthanum strontium manganese (LSM) is also being investigated, which avoids some issues with nickel oxidation and degradation.
- **O_2 electrode**: LSM is used on the oxygen side electrode, research has involved combining with nanoparticles to prevent delamination, where the material fractures into layers.

While solid oxide electrolysers are currently at a lower technology readiness level than alkaline or PEM electrolysers, development of this technology may be beneficial given the potential advantages available. Solid oxide electrolysers can operate at higher electrical efficiencies than PEM or alkaline electrolysers, by using thermal energy to promote electrolysis. By coupling solid oxide electrolysers to a source of high temperature heat, such as from nuclear power or solar heat generators, solid oxide electrolysers will be able to produce more hydrogen per kWh of input energy than other electrolyser types.

Solid oxide electrolysers can operate reversibly as both an electrolyser and a fuel cell. In a decarbonised energy system this dual functionality means solid oxide electrolysers can either generate electricity or produce hydrogen. This hydrogen could be stored, offering the potential to act as an electricity grid balancing mechanism.

Case study: UK solid oxide electrolyser expertise

The academic and industrial experience in the UK could be built on to develop solid oxide capability – organisations such as Ceres Power, Rolls-Royce, Imperial College and the University of St Andrews all have experience in this area.

Solid oxide electrolysers can produce carbon monoxide from a carbon dioxide input, in the same unit that produces hydrogen from steam. This 'co-electrolysis' unit would therefore produce syngas, a key feedstock that may be used to produce a number of common industrial chemicals such as methanol, and hydrocarbon fuels through Fischer-Tropsch synthesis. Co-electrolysis typically results in faster rates of electrolyser degradation (<5%/1,000 hours), and therefore presents a challenging research topic [19].

Marinization of electrolysers through corrosion resistant materials

Offshore electrolysis presents various challenges including the need for compact, low maintenance, vibration-tolerant designs, acquiring sufficient pure water via desalination along with several other operational requirements. From a materials perspective, there is a need to develop electrolyser systems capable of long-term operation in harsh marine environments.

A number of offshore hydrogen production projects have been announced over the past 12 – 18 months [20] [21] [22] [23], whereby electrolysers are linked to offshore wind turbines to produce renewable hydrogen. Undertaking any engineering project offshore is more difficult and costly than working on land, and in general in the energy sector efforts are made to minimise and reduce the complexity of any equipment that must be located offshore. Locating electrolysers offshore appears to go against this principle when they could be sited on land and connected to offshore wind turbines via sub-sea cables. However, in establishing the lowest cost solution for wind-to-hydrogen systems there are multiple factors to consider, including the cost of production and transport of electricity versus hydrogen. Moving energy in the form of hydrogen could potentially be more cost effective, especially for sites far from land if existing gas pipelines could be repurposed to transport hydrogen. The economics of offshore hydrogen production were examined in the 2020 study by the Offshore Renewable Energy Catapult [24].

As of early 2021, offshore hydrogen production remains at the feasibility / design stage; to the authors' knowledge there are no examples of electrolysers installed and operated in offshore environments to date. A recently announced EU-funded project will develop a marinized MW-scale electrolyser system and complete a period of testing in a representative shore-side environment [25], in preparation for offshore deployment later in the decade.

Photocatalysts for direct water splitting

Direct solar water splitting uses a photocatalyst under direct sunlight to split water into hydrogen and oxygen. Photocatalyst materials are currently at a low technology readiness level. New, stable materials are required that would need to be able to utilise visible light to split water if they are to offer effective solar-to-hydrogen conversion.

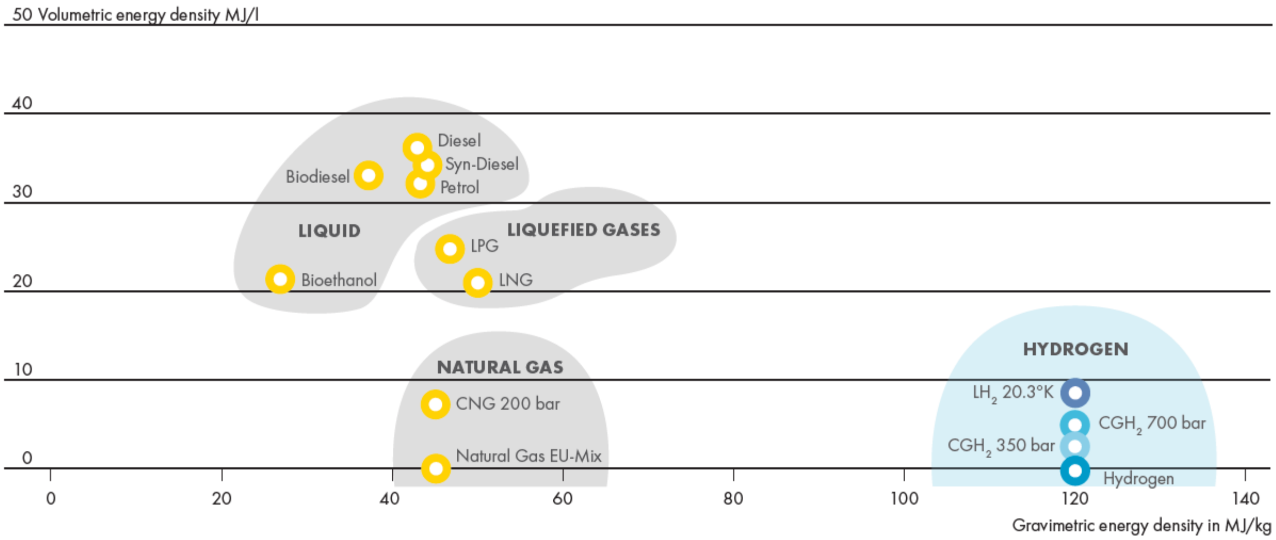
Materials such as strontium titanate can split water using UV light, and have been shown to have relatively high efficiency and stability [26]. However, high efficiency solar-to-hydrogen devices will only be achieved using visible light to split water, since UV light accounts for only 5% of the energy in solar radiation, whereas 50% of solar energy is comprised of visible light [26]. While this technology has advanced significantly over recent years, further improvements to material stability and efficiency are required. Computational design of materials can support the design of new materials for solar water splitting [27] – this topic is covered in section 6.

Significant research and innovation will be required to increase photocatalyst activity and stability before solar water splitting devices may be tested at scale, over long periods. Due to this low level of technology readiness solar water splitting is a long-term research goal, but it could be a disruptive technology if efficient and low-cost materials are developed. Deployment opportunities are likely to lie outside the UK.

3. Hydrogen storage and distribution

Introduction

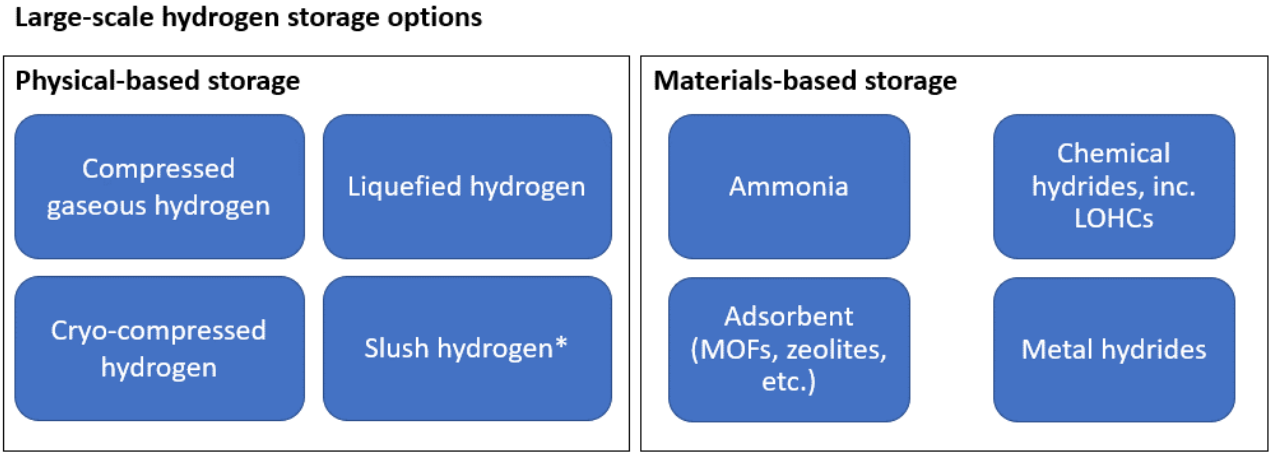
One of the benefits of hydrogen is the potential it offers for long-term storage of energy at scale. However, the physical and chemical properties of hydrogen lead to higher storage and transportation costs relative to other energy carriers such as liquid hydrocarbon fuels (diesel, bioethanol, etc.). The graph below shows the gravimetric (energy per unit mass) and volumetric (energy per unit volume) energy density of hydrogen in various states, relative to a selection of other liquid and gaseous fuels (based on lower heating values).



Source: Shell Hydrogen Study [28]

The figure demonstrates that while hydrogen has a high gravimetric energy density, its volumetric energy density is much lower than liquid fuels. For practical applications it is necessary to find ways of storing sufficient quantities in manageable volumes by increasing the density of hydrogen.

The principal hydrogen storage methods used to date are physical-based solutions in which hydrogen is compressed and / or cooled. Various materials-based storage technologies are also under development and being investigated by the academic community. The main options are summarised in the figure below.



LOHC: liquid organic hydrogen carrier, MOF: metal organic frameworks

* Slush hydrogen is a combination of liquid and solid hydrogen at the triple point (primarily investigated as a fuel for space travel).

A detailed description of the options for hydrogen storage and distribution is available in the literature [29] [30].

A key benefit of using hydrogen as an energy carrier is the ability to transport it using the existing natural gas grid infrastructure. This could be a key enabler for increased hydrogen uptake in energy applications, providing a practical and cost-effective way of transporting large amounts of energy. Research topics examining hydrogen distribution using the existing gas grid infrastructure are a key focus area for the UK.

Three key materials research challenges to support the storage and distribution of hydrogen have been identified:

- **Improving catalysts for distributed ammonia production and cracking**, which will enable hydrogen to be stored and distributed at scale as ammonia and converted back to hydrogen at the point of use.
- **Improving point of use hydrogen purification technologies**, so that large-scale hydrogen use in fuel cells can be enabled through gas grid distribution.
- **Detailed understanding of material degradation pathways for high volume compressors**, to ensure high pressure hydrogen compression at scale is consistent with appropriate compressor service life, to enable gas grid distribution.

These key research priorities are discussed below, while further research challenges are discussed in the second part of this chapter.

Key materials research challenges

Key priority: Improving catalysts for distributed ammonia production and cracking

Ammonia may be used as a hydrogen carrier, due to its relatively high density at moderate temperatures (compared to liquid hydrogen), and as an industrial feedstock. To support the use of ammonia as a hydrogen carrier at scale requires the development of efficient catalysts that allow ammonia to be produced on a distributed scale, and to enable ammonia be cracked more efficiently into hydrogen and nitrogen.

The relatively high density, efficiency of conversion, and moderate liquefaction temperature of ammonia has made it a key hydrogen carrier candidate. Given ammonia is already transported around the globe as an industrial feedstock, existing logistics and engineering know-how can be exploited to optimise the distribution of ammonia. Ammonia can be liquefied at a higher temperature than hydrogen, and liquid ammonia has a hydrogen volumetric density of 107 kg/m^3, and gravimetric density of 17.6 wt.% [31]. This high energy density has made ammonia of interest for applications where large quantities of hydrogen would be required, such as in shipping.

A significant proportion of hydrogen produced today is used in ammonia manufacture through the Haber-Bosch process. While this process has been established in industry for many years, work continues to improve catalyst performance. A less common research topic is the development of solutions to allow smaller-scale, distributed ammonia production with a lower carbon footprint. One option would be to produce ammonia directly from electrolysis. This will require the development of new electrolyser systems, including electrolytes, anode, and cathode materials. Production of ammonia from electrolysis was recently achieved by researchers at the University of Illinois at Chicago and the University of Minnesota, where 300mg of ammonia was produced from a nitrogen reduction reaction [32]. This technology is currently at an early stage and significant work will be required to optimise and scale up the process, requiring new materials developments.

In applications where ammonia is used as a storage mechanism for hydrogen, the ammonia will need to be 'cracked' back into hydrogen and nitrogen. Catalysts for this reaction have not been developed to the same extent as those for the Haber-Bosch process. While ruthenium, and nickel and iron-based systems are expected to be beneficial for ammonia cracking, recently the UK Science and Technology Facilities Council (STFC) developed a new family of catalysts that may be suitable, comprised of metal amides and imides [33]. These catalysts were able to reduce the cracking temperature by 50°C, offered improved performance under thermal cycling, and are expected to have significantly lower cost than ruthenium-based catalysts. While research is ongoing to scale up systems based on these catalysts, it remains a promising discovery for the UK.

Key priority: Improving point of use hydrogen purification technologies

Hydrogen can be effectively distributed using existing gas grid infrastructure, reducing the cost of hydrogen distribution, and allowing gas grids to transition to a net zero future. Given that hydrogen leaving the grid will be at relatively low purity, and hydrogen fuel cells currently require high levels of hydrogen purity (>99.97%[2]), improvements are required in downstream purification technologies close to point of use. Leading materials-based solutions include the use of membranes and pressure swing adsorption.

When hydrogen production is not co-located with the source of demand, it is currently transported from production sites to end uses (such as hydrogen refuelling stations for fuel cell vehicles) by tube trailer in most cases. Gaseous tube trailers can carry around 300 – 900 kg of hydrogen [34]. While this is a relatively large amount of fuel compared to the size of existing hydrogen refuelling stations (typically with capacity of low hundreds of kilograms per day), there is a trend towards larger capacity refuelling stations for heavy duty vehicles. Designs are emerging for hydrogen refuelling stations with a capacity of multiple tonnes per day [35], for which delivery of hydrogen via tube trailer in either gaseous or liquid form will become increasingly impractical. While various other solutions are available, using existing gas grids to transport hydrogen from centralised production sites to strategically placed hydrogen refuelling stations is potentially an attractive option.

Given the number of UK projects examining the possibility of hydrogen blending in the gas grid (Hy4Heat, HyNet, FutureGrid, and H21) there is a need to develop solutions to allow hydrogen from the UK gas grid to be used in fuel cell applications.

There are two potential places where hydrogen purity for fuel cell applications can be dealt with:

1. By purifying hydrogen from the gas grid at the point of use
2. By increasing fuel cell tolerance to impurities

This topic under examination here concerns purification at the filling station, for which several materials-based separation technology options exist. The challenge of improving fuel cell tolerance to impurities is covered in section 4. The most promising materials solutions for hydrogen purification – on the basis of cost, scalability, and technology readiness – are membranes and pressure swing adsorption.

The most common hydrogen purification technology is currently pressure swing adsorption (PSA), in which the gas stream is passed over an adsorbent material, which captures impurities. The pressure of the system is cycled to regenerate the adsorbent material. This method allows transport-purity hydrogen to be produced, however significant costs are introduced due to the relatively low hydrogen recovery of circa 90% owing to ~10% losses on system purging [36]. PSA units typically contain materials such as zeolite 5A, silica gel, alumina, and activated carbon. Metal organic framework (MOF) based materials may also be used for PSA in the future [36]. New materials would aim to improve hydrogen recovery by increasing the binding between the adsorbent material and the impurity molecules.

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[2] Maximum allowable concentration of a variety of impurity chemicals has been set out in the ISO standards for hydrogen for PEM fuel cells [48]

Case study: Developing UK expertise on materials for hydrogen purification.

Linde and Evonik have collaborated on a combined polymer-based membrane and PSA system, designed to be used at hydrogen refuelling stations supplied by the gas grid, with a full-scale demo plant due to go online in 2021 [57]. The UK has significant academic expertise in hydrogen purification, with research on membranes at the University of Birmingham and PSA at the University of Edinburgh.

Membranes that selectively allow hydrogen to pass through could be used to purify hydrogen from the gas grid at the point of use, either in combination with PSA or as a standalone solution. Palladium-based membranes have been tested at small scale (3.6 kg/hour), but the current operating temperatures of 300 – 600°C make operation as part of the gas grid impractical [37]. Polymer-based membranes are also available, however are unable to achieve the level of purity required for fuel cell applications [36]. These membranes could be combined with other purification technologies to achieve sufficiently high purity levels. Membrane cost is particularly challenging since the failure of a purification membrane at the point of use could cause significant damage to fuel cells. Gas network operators suggested installation of multiple membranes to provide redundancy should costs be low enough. Several approaches to lowering the cost of palladium-based membranes exist, for example including Pd-alloy thin films on porous supports, and the use of transition-metal-based amorphous alloys to replace palladium. Materials research challenges for hydrogen separation membranes include ensuring high selectivity, resistance to impurities such as sulphur, and mechanical and thermal stability, while also achieving a high rate of hydrogen transfer across the membrane. The rate of hydrogen transfer and capital cost are optimised by reducing membrane thickness, but thinner membranes allow increasing quantities of impurities to pass through. There is therefore a clear materials optimisation challenge to improve these membranes.

Key priority: Detailed understanding of material degradation pathways for high volume compressors

Transport of hydrogen in the gas grid will require the use of gas grid compressors, to take hydrogen to the pressures required for transmission (up to 94 bar) and distribution (16 bar). The small size and light weight of hydrogen molecules, along with its ability to degrade materials, through mechanisms such as hydrogen embrittlement and high temperature hydrogen attack [38]*, makes the design of hydrogen compressors particularly challenging*.

Reciprocating and diaphragm compressors (positive displacement type) are most commonly used to compress hydrogen in industry and for transport purposes. Centrifugal compressors often have mechanical design and efficiency advantages over positive displacement compressors in high flow rate, <100 bar outlet pressure applications found in gas transmission networks. Reciprocating and diaphragm compressors are currently used at hydrogen refuelling stations to compress hydrogen from electrolysers (10s of bar) or tube trailers (250 – 500 bar), to refuelling pressures up to 700 bar. Centrifugal hydrogen compressors are comparatively less mature, as work is currently ongoing to design and build prototypes compatible with high flow rate applications [39].

For centrifugal compressors, the low weight of hydrogen molecules means the impeller blades tips operate at speeds around three times faster than for other gases, in order to achieve the same pressure differential. This leads to large amounts of heat dissipation and a need for materials that can withstand high temperatures and mechanical stresses in a hydrogen-rich environment.

Previous studies on the design of centrifugal hydrogen compressors indicate that commercially available high-strength steel and titanium alloy materials have the yield and fatigue strength properties to be used as impellers in centrifugal hydrogen compressors [40]. These studies recommended a coating be used on compressor materials to prevent hydrogen embrittlement and other degradation mechanisms while critically not impacting the material properties of the base material. Several coatings candidates have been proposed [39], but greater understanding of materials degradation in real-world environments over the long term is required.

The poor understanding of compressor materials degradation in real-world environments leads to challenges with materials selection and inspection protocols. The need to develop standardised materials inspection protocols and understand hydrogen degradation mechanisms is discussed in section 6.

Understanding degradation mechanisms for hydrogen compressors is key to determining whether existing gas grid compressors may be used when hydrogen is injected into the gas grid, or whether new compressors will be required. New compressors will incur significant additional costs and impact the timescales for hydrogen transport in the gas grid.

In the longer term, compressors based on materials capable of storing hydrogen and releasing it at increased pressure under a thermal cycling mechanism, such as adsorbent or metal hydride materials compressors, may be able to provide solutions. While this mechanism is significantly less efficient than traditional positive displacement or centrifugal compressors, it benefits from using a heat energy input, and therefore could be exploited at industrial sites where large quantities of low-grade waste heat is generated.

Given the number of UK projects examining the potential to blend hydrogen into the gas grid and the need for the UK to develop material testing capability and expertise on hydrogen degradation mechanisms, this represents a key area.

Further materials research challenges

Beyond these key priorities there are a number of other research topics of interest to support the storage and distribution of hydrogen. The first covers testing existing gas pipeline materials and gas grid components for hydrogen compatibility, where research is already showing promising results. The other topics on liquid hydrogen storage, adsorbents, and metal hydrides aim to reduce the cost and improve the capacity of hydrogen storage.

Testing existing pipeline materials and components

To allow hydrogen transmission through the existing gas networks, the impact of hydrogen on existing pipeline materials and component properties must be understood, to prevent damage to infrastructure when hydrogen is distributed through the gas grid. Several projects are examining the compatibility of the existing gas network with hydrogen blending in the UK, such as HyNet, FutureGrid, and H21.

Currently several different pipeline testing methodologies are used to test the impact of hydrogen blending on pipeline materials. There is a need for standardisation of testing and inspection protocols for materials research to support research activities; this is discussed in section 6.

Testing indicates that certain existing pipeline materials are incompatible with hydrogen blending in the gas grid due to hydrogen embrittlement. The impact of hydrogen embrittlement is expected to be more significant in high pressure transmission networks, compared with lower pressure distribution networks. New pipeline materials, based on polymers, are not impacted by hydrogen distribution in the gas grid. Gas grid operators have flagged the importance of understanding the implications of hydrogen on any pipeline joints and downstream components within the gas grid, such as valves, regulators, and springs, to determine the lifetime impact of hydrogen on their properties. Some components may need to be replaced with new materials or materials with coatings that are resistant to hydrogen embrittlement and other degradation mechanisms under mechanical cycling.

Materials for liquid hydrogen storage tanks

Hydrogen can be liquefied at -253^{o}C to achieve 71 kg/m^3 volumetric density, for distribution and potentially heavy-duty on-board storage applications, particularly for maritime and aerospace sectors. This results in a need for tank materials that can exhibit high strength, stiffness, and fracture toughness in hydrogen-rich and extremely low temperature environments [41]. *Further, insulating materials are required to minimise hydrogen losses through boil-off. There is a significant energy penalty associated with storing hydrogen in liquid form.*

Candidate materials for liquid hydrogen storage tanks include monolithic metals, continuous-fibre-reinforced polymer matrix composites, and discontinuous reinforced metallic composites [41]. Different applications may require different material properties, e.g. minimising weight is a key priority for aerospace applications.

To minimise heat-transfer to liquid hydrogen, the tank is insulated with materials kept in a vacuum, since gases in air condense or solidify at the temperature of liquid hydrogen. These materials should have low thermal conductivity and diffusivity. Polymer foams, aerogels, and multi-layer insulation systems are promising candidates for this application [41].

Given the low temperatures of liquid hydrogen tanks, both tank and insulation materials should have low coefficients of thermal expansion that are compatible with other tank materials. Improvements in materials design are expected to lead to significant weight reductions for liquid hydrogen tanks by improving materials selection and reducing safety margins through greater understanding. This will facilitate the use of liquid hydrogen in aviation applications.

Adsorbent materials for hydrogen storage

Metal Organic Framework (MOF) storage can be optimised by maximising surface area and porosity. MOF analysis suggests that their volumetric capacity is limited to 40 kg/m^3 [42], *compared with 70kg/m^3 for liquid hydrogen, or 107kg/m^3 for ammonia. Significant breakthroughs in these materials will be required to reach comparable storage capacity to liquid hydrogen or ammonia.*

Adsorbent storage commonly focuses on metal organic frameworks (MOFs), a linked framework comprising metal ions surrounded by organic 'linker' molecules. This hollow structure gives the materials a very high surface area, suitable for storage of gases such as hydrogen. MOFs store hydrogen using a physisorption mechanism, whereby hydrogen molecules are loosely bound to the material surface. To increase the hydrogen capacity of the material, it is cooled, and the stored hydrogen is then released on heating.

In the short term, it is likely absorbent hydrogen storage will remain challenging at ambient temperature, however, adsorbent storage can achieve better energy density than cryo-compressed hydrogen at temperatures above -196°C. This is a significant advantage, as cooling to these temperatures can be achieved at much lower cost than those required for liquid hydrogen (-253°C).

MOFs can be screened using computational methods. Work is now being undertaken to optimise MOF properties using machine learning, with predictive algorithms potentially able to indicate which structures will offer improved hydrogen storage properties. The application of artificial intelligence to materials research is discussed in section 6.

Case study: UK research on MOFs

Research on MOFs is being carried out at a number of academic institutions across the UK, including the University of Birmingham and the University of Bristol.

Metal hydrides for hydrogen storage

Metal hydrides can reversibly store hydrogen under a temperature or pressure swing, with an operating temperature range of 20°C – 100°C. Different metal hydride compositions operate at different temperatures and pressures, and materials research will optimise metal hydride composition to minimise cost, improve recyclability, and crucially, maximise hydrogen storage capacity for different applications.

Improving the storage capacity of metal hydrides to compete with gaseous or liquid hydrogen at scale while maintaining an acceptable cost has been challenging. There are reports of some demonstration material systems.

A paper published by researchers at Lancaster University in 2019 indicates that a reversible excess adsorption performance of 10.5 wt.% and 197 kgH$_2$ m^{-3} at 120 bar at ambient temperature was achieved by a novel manganese hydride material [43]. By comparison, current gaseous storage tanks for on-board hydrogen storage at 700 bar are able to achieve capacities of 4.2 wt.% and 24 kgH_2 m^{-3} [44]. While the performance of this material has thus far only been demonstrated at a milligram scale in a lab environment, if proven at scale it would exceed the performance of any other hydrogen storage technology to date. Although significant further research is required to confirm these results, this material could represent a breakthrough for both on-board, trailer, and stationary storage.

A magnesium hydride based 'POWERPASTE' has been developed by the Fraunhofer Institute, that is able to store hydrogen at ambient temperature and pressure and release it when reacted with water [45]. Cannisters of the paste are expected to provide an on-board hydrogen storage option for e-scooters, drones, cars, delivery vehicles and other options. A demonstration production site is set to start producing up to 4 tonnes/year of POWERPASTE per year in 2021 [45]. This type of material could be used to reduce the cost of the hydrogen refuelling infrastructure and allow hydrogen to be used in new vehicle types.

4. Hydrogen use in transport

Introduction

The main options available for decarbonising the transport sector include the use of direct electrification with battery electric drivetrains, biofuels (likely to be relatively limited due to resource constraints and demands for biofuels in other sectors), and the use of renewable hydrogen and hydrogen-derived synthetic fuels. Each option has pros and cons, with some better suited to certain applications and duty cycles than others. There is a strong focus on direct electrification of transport as the primary means of achieving emissions reduction in the short term. Based on current technology, battery electric solutions cannot provide a like-for-like replacement for all transport modes. It is accepted that a portfolio of technologies is likely to be required to achieve full decarbonisation of the transport sector, including hydrogen fuel cell options for heavy duty or long range transport.

Key materials research challenges

Key priority: Materials-led solutions for cost-effective, conformable tank hydrogen storage in fuel cell vehicles

Hydrogen-powered vehicles currently use gaseous hydrogen stored at 350 or 700 bar pressure in cylindrical vessels. Hydrogen storage tanks are the most expensive component in current hydrogen fuel cell cars [46] *and add significant weight. Cylindrical shapes are used to achieve a more uniform distribution of forces, allowing the storage of high-pressure gas while minimising the risk of cracks and failures. The low packing efficiency of this shape creates challenges to achieve the required hydrogen storage in a limited space. Materials led solutions offering more conventional fuel tank shapes would allow optimal use of on-board space and greater flexibility in vehicle design*.

Current hydrogen vehicles use either type III tanks, which are made from a metal liner wrapped by a composite material to provide strength, or type IV tanks, made from a plastic liner with a composite wrap. Alternative materials such as new polymers or resins, as well as different approaches to manufacturing could reduce the cost of gaseous storage tanks for on-board storage. Large scale manufacture of gaseous hydrogen storage tanks will reduce cost further through economies of scale from streamlining and automation of manufacturing, reducing the cost of materials and components through large-scale procurement, and other efficiencies. The life cycle of the storage tanks also needs to be considered.

Research on hydrogen tank materials needs to be aligned with manufacturing of the overall storage system, to ensure that fittings are compatible with hydrogen and the new tank materials developed. Beyond type IV tanks, the mass and cost of storage tanks may be improved by removing the liner, use of resins, reinforcements, additive technologies, and filament winding and braiding technologies.

Case study: UK expertise on composite materials

The UK has significant expertise in composites through institutions such as Imperial College and the National Composite Centre, which could be exploited to develop lower cost conformable composite tanks.

Further work will be required to support the development of materials for low-cost, conformable hydrogen tanks; in particular the development of UK testing capability, a standardised approach to lifecycle analysis, standardised testing and inspection protocols, and end-of-life treatment. These enabling topics are discussed further in section 6.

Further materials research challenges

Further materials challenges for hydrogen transport, that while not key research priorities, are important to support hydrogen use in transport, are listed below. These topics largely focus on reducing cost and improving the operational viability and life cycle impact of PEM fuel cells, which are the incumbent technology used in fuel cell vehicles today. These topics include:

- Reducing loading of scarce (and expensive) materials in PEM fuel cells.
- Removing fluorine from PEM fuel cell membranes, which has negative environmental impacts.
- Improving fuel cell tolerance to impurities, to reduce the cost of hydrogen purification.
- Improving the material stability and lifetime of solid oxide fuel cells.

Reducing loading of scarce materials in PEM fuel cells

The use of platinum in fuel cells leads to materials research challenges on two timescales: first, in the near-term platinum loading should be minimised by increasing the active catalyst area and mitigating catalyst degradation. Second, in the longer term the development of new catalysts for use in vehicle fuel cells could enable platinum to be removed entirely from vehicles.

The current fuel cell technology of choice for vehicle applications is the proton exchange membrane (PEM) fuel cell, which offers low temperature operations and faster response than other technologies. PEM fuel cells are composed of a polymer membrane covered by a platinum catalyst on both sides, between an anode and cathode. The platinum, in the form of nanometre-sized particles, catalyses the splitting of hydrogen molecules into protons and electrons on the anode side, and oxygen reduction on the cathode side. Unlike polymer electrolyte membrane (PEM) electrolysers, PEM fuel cells do not contain iridium.

While platinum is the best material available to be used as a catalyst in this reaction, high platinum loading in fuels cells leads to increased cost. Moreover, platinum catalysts suffer from poisoning by impurities in hydrogen and other degradation mechanisms. Fuel cell manufacturers indicate that 20–40% additional platinum must be used to ensure that fuel cell performance is adequate for the entire vehicle lifetime. This results in high levels of demand for platinum of 30g for an 85kW engine of a fuel cell car [47]. The goals stated in the Hydrogen Council's scaling up report - a target of 10 to 15 million fuel cell cars on the road by 2030 [6] - would require around 2 years of the 200 tonnes/year of global platinum production capacity [3] for fuel cell cars alone. Once other vehicle types are accounted for, it seems likely that platinum loading within fuel cells may place limits on the number of fuel cell vehicles that can be manufactured. Targets have been set, for the mass of platinum group metals in a fuel cell. The benchmark is the quantity of precious metal currently used in a catalytic convertor for vehicles with an internal combustion engine.

While some non-scarce metal catalysts for fuel cells are being investigated based on iron, nitrogen, carbon, or molybdenum disulphide, transport requires high current densities that cannot yet be achieved by non-scarce metals, limiting these catalysts to low-power applications.

Fortunately, technologies are currently available that can recover precious metal catalysts from fuel cells at the end of their life, and therefore scarce metal catalysts can be used sustainably as part of a circular economy. It is worth noting that the demand for certain scarce metals will change significantly in a decarbonised energy system, where internal combustion engine vehicles are replaced with battery or fuel cell alternatives. The demand for platinum, palladium, and rhodium for catalytic converters for road vehicles will be reduced. It is estimated that 70 tonnes of platinum production per year is currently used in conventional catalytic converters [47], which could be used in fuel cells in a decarbonised transport system.

Removing fluorine from membranes in PEM fuel cells

Currently, the only candidate for PEM fuel cell membranes is Nafion, an ionomer that requires fluorine in the manufacturing process. A long-term goal for reducing the environmental impact of fuel cell manufacturing is to develop new membrane materials that do not require fluorine, or other environmentally damaging chemicals, to manufacture.

PEM fuel cells contain a membrane that allows protons to diffuse from the anode to the cathode, generating an electrical current in the process. To maximise fuel cell efficiency, these membranes must be thin to minimise ionic resistance, however thin membranes can suffer from gas crossover, whereby hydrogen molecules cross the membrane leading to reduced fuel cell efficiency, or low durability.

Any candidate membrane materials will need to have low ionic resistance and be sufficiently durable within the harsh conditions of a fuel cell. Since few promising candidate materials are available, this is expected to be a longer-term research challenge.

Improving fuel cell vehicle tolerance to impurities

Currently, PEM fuel cells require very high hydrogen purity of >99.97% [48] *and will experience significant loss in performance if exposed to higher concentrations of impurities in the fuel.*

Transporting hydrogen in the gas grid will result in entrainment of impurities leading to insufficiently pure hydrogen at the refuelling station. One solution is to improve the tolerance to hydrogen impurities of fuel cells for mobility applications. This would reduce the cost of hydrogen, enabling it to be transported within the gas grid, while reducing purification requirements at hydrogen refuelling stations. This is a long-term research challenge, since PEM fuel cells are currently very sensitive to impurities and routes to increasing their tolerance are not yet mature research topics. It is possible that some combination of on-board monitoring, use of diluants, and increased fuel cell tolerance to impurities will enable relaxation of the requirements for purification at hydrogen refuelling stations.

Fuel cell vehicles also require air intake filtration, requiring on-board filters that are regularly replaced, as impurities can poison fuel cell catalysts and thus reduce vehicle performance. Due to varying levels of air pollution, predicting when these filters will need to be changed is challenging, and there is no indicator of when a filter is at the end of its lifetime. Filters could be improved by reducing cost and improving durability to increase their lifetime. Development of on-board sensors to determine when a filter needs to be replaced would also be beneficial to vehicle users.

Solid oxide fuel cells

In the long term, solid oxide fuel cells have the potential to be used for certain transport applications [49]*. The high operating temperature (600°C - 1,000°C) of solid oxide fuel cells can, however, be a disadvantage for transport applications since vehicles would have a slow start up time and protection from heat would be required for both drivers and passengers* [50]*.*

Case study: development of UK expertise on solid oxide fuel cells

Solid oxide fuel cell technology is still relatively early stage and would be a longer term solution, however it is an interesting area of research for the UK, which is already strong in this topic with expertise at University of St Andrews, and UK-based fuel cell and engineering company Ceres Power.

The high temperatures used in solid oxide fuel cells cause the rapid degradation of materials within the fuel cell. New materials are required that will allow solid oxide fuel cells to operate at lower temperature (400°C – 600°C) in the next generation of solid oxide fuel cells [51].

Like solid oxide electrolysers, solid oxide fuel cells commonly use an yttria-stabilized zirconia electrolyte, which exhibits high ionic conductivity at high temperatures (>600°C). Materials research is therefore needed to develop a low cost electrolyte which exhibits high ionic conductivity at reduced temperatures, to reduce materials degradation. Anode materials must be thermally stable, electronically conductive, and able to act as an electrocatalyst at lower temperatures. Hussain and Yangping explore a number of candidate materials for a solid oxide fuel cell electrolyte, anode, and cathode in their 2020 paper [52].

In 2016, Nissan demonstrated a prototype passenger car capable of running on bio-ethanol. An on-board reformer is used to produce hydrogen. The hydrogen is then supplied to a solid oxide fuel cell [53]. Systems such as this could allow a wide variety of fuels to be reformed on-board to provide power for vehicles.

5. Hydrogen use in heating and power generation

Introduction

Hydrogen can be used in domestic boilers and industrial burners either as pure hydrogen or blended with natural gas. In industry, the CO_2 emissions associated with the production of steel, gas, cement, and ceramics could be reduced by using low-carbon hydrogen for heat, instead of natural gas.

Hydrogen can also be used to generate electricity through gas turbines or fuel cells. This could provide balancing services to the electricity grid on a variety of timescales (from hourly to seasonal) within a decarbonised energy system. The UK is conducting research in this area through programmes such as Hy4Heat and HyNet.

While none of research topics in this area met the criteria to be classed as one of the top five ‘key materials research priorities, hydrogen is likely to play a role in decarbonising industry, domestic heat, and the power sector. The topics within this sector may emerge as research priorities over time. Research challenges in this area include:

- Understanding the impact of hydrogen heating on industrial products
- Developing materials for hydrogen-fired kilns and furnaces
- Understanding hydrogen degradation mechanisms in gas turbine blades
- Developing materials for hydrogen burner nozzles

Materials research challenges

Understanding the impact of hydrogen heating on industrial products

Industrial processes to manufacture ceramics, glass, and steel use direct firing to heat equipment, whereby gases are combusted inside the furnace to provide process heat. For these processes, it will be crucial to ensure the properties of the resulting products are not negatively impacted by hydrogen combustion to heat the furnace.

Changes in the properties of industrial products when switching to hydrogen from natural gas heating could result from chemical reactions between impurities, changes to flue gas composition, or the different combustion temperature and thermal transfer properties of hydrogen.

Hydrogen combustion results in a higher water content in furnace flue gases, the impact of which on the properties of glass and ceramics are unknown. The raw materials used to produce ceramics can contain fluorine, and hydrogen may contain impurities such as sulphur compounds, both of which may cause changes to the properties of the final products. Testing the properties of materials produced using direct-fired hydrogen heating through demonstration projects, and if necessary, finding ways to mitigate the impact of hydrogen heating on materials properties will be necessary to facilitate the roll-out of hydrogen for industrial heat applications.

Case study: hydrogen for industrial heat demonstrations in the UK

Demonstration projects for industrial fuel switching to lower carbon alternatives are already going ahead in the UK, with organisations such as Glass Futures working to demonstrate the use of hydrogen (among other solutions) in the glassmaking process [60], and a trial of green hydrogen for process heating is going ahead at a cement plant in Wales [59]. Several UK universities have academic expertise in testing the impact of hydrogen heating on industrial products, such as Surrey, Birmingham, Sheffield Hallam, and Imperial College. Lessons learnt from demonstrations in the glass and cement industry should be linked to the use of hydrogen heating in other industries, such as ceramics.

Materials for hydrogen-fired kilns and furnaces

Refractory materials are employed in kilns and furnaces to insulate and prevent degradation of the kiln or furnace. These materials operate for long periods under high temperature cycling, often under high pressures, and in corrosive chemical environments. They must be able to retain their shape and strength over their lifetime in these environments.

Use of hydrogen may impact the degradation rates of refractory materials due to the different temperature, heat transport properties, or gas composition. Before hydrogen can be used as a long-term furnace heating solution, the impact of hydrogen heating on refractory material degradation must be tested. Suitable solutions will need to be developed should materials be shown to degrade significantly faster.

Materials and coatings for hydrogen gas turbine blades

The use of hydrogen in gas turbines will cause challenges due to low density, potential for hydrogen embrittlement, high temperature hydrogen attack, and high-water content of the flue gas. Research will be needed to understand degradation mechanisms for gas turbine materials under these conditions.

In a fully decarbonised economy, fast response peaking plants may be needed to run on low carbon fuel, rather than the natural gas turbines used today. Hydrogen turbines could be used to provide decarbonised rapid response electricity generation.

Turbines operating with any fuel experience extreme temperatures, corrosive environments, and mechanical stresses. At temperatures above 400°C, steel becomes sensitive to a high temperature hydrogen attack, whereby hydrogen dissociates, dissolves in steel, and reacts with carbon in the steel to form methane [38]. Depending on the severity of this degradation, it can lead to a significant degradation in material properties.

Case study: Developing UK hydrogen gas turbine capabilities

Companies such as Mitsubishi Heavy Industries, GE, and Siemens have demonstrated gas turbines able to use blends of hydrogen and natural gas as fuel, and are working towards development of turbines capable of running on 100% hydrogen fuel [63] [64] [62]. Equinor and SSE Thermal have developed plans for a hydrogen-fuelled power station in the Humber that is expected to come online by the end of the decade (dependent on policy support from the UK government) [61]. This would be the world's first major 100% hydrogen-fired power plant station, with 1,800MW of peak capacity, positioning the UK as a global leader in power from hydrogen.

Research is still required to understand degradation mechanisms in hydrogen turbines, and how materials operating in these conditions may be inspected. This links to the enabling topic on inspection procedures in section 6.

Materials for hydrogen burner nozzles

To enable hydrogen use in industrial heating, burner nozzles will need to be resistant to hydrogen embrittlement, high temperature hydrogen attack, and any other hydrogen degradation mechanisms that are present at extreme temperatures.

Hydrogen has a faster flame speed than natural gas, leading to higher local flame temperatures. This can result in NOx emissions, if combustion is not carefully controlled. New burner designs and geometries will be required, to minimise NOx emissions from hydrogen burners and boilers by optimising the rate at which hydrogen and oxygen mix [54] [55] [56]. Materials testing and development in this area should consider the design of hydrogen-specific burners. The development of UK capabilities in standardised materials testing protocols is discussed in section 6.

6. Research and technology enablers

In addition to the specific research topics outlined in the earlier sections, there are some key enablers that will increase the impact and uptake of materials research. These are:

- **Creating consistent lifecycle analysis approaches and data sets** - developing consistent definitions and approaches alongside transparent and accessible databases to support lifecycle analysis of materials for hydrogen use and ensure the complete materials footprint is understood.
- **Improving end-of-life treatment of materials –** designing products for end of life to enable materials recovery and reuse, and minimise waste creation.
- **Developing UK capability to test, set standards, and accredit new materials -** developing standardised testing methodologies to allow comparison of experimental results, and understanding materials degradation mechanisms, to develop testing and inspection protocols to provide ongoing safety assurance for hydrogen materials.
- **Computational design of materials -** using artificial intelligence to lead the design of materials with specified properties and accelerate the discovery of candidates, leading to rapid results and new materials insights.

While these topics are important to support all materials research, they have particular relevance to materials for hydrogen. Case studies of the applications of these enablers to support materials for hydrogen are provided for each topic to demonstrate the importance of these topics.

Creating consistent lifecycle analysis approaches and data sets

When creating materials solutions to support the decarbonisation of various energy systems, it is crucial to understand the full lifecycle impact of those materials and for researchers to be able to follow consistent methodologies and data sets in conducting these assessments.

The establishment of consistent lifecycle analysis approaches will enable resources to focus on areas that deliver the most effective emissions reductions. To enable materials researchers to compare different material lifecycle impacts, consistent approaches to lifecycle analysis and transparent, and standardised emissions data sets must be developed.

Lifecycle analysis case study: low carbon hydrogen production

Consistent approach to lifecycle analysis is particularly important in allowing governments and industry to evaluate the emissions associated with various hydrogen production pathways. The carbon emissions generated in producing, for example, electrolytic hydrogen, including the impact of rare metal production and the source of electricity need to be evaluated so that genuinely low carbon hydrogen pathways can be supported.

Improving end-of-life treatment of materials

Materials to support the production, storage, distribution, and use of hydrogen should be designed with circular economy principles in mind. Namely, to reduce waste and find ways to reuse and recycle existing products.

While materials recovery is currently implemented for high-value metals used as catalysts, this is often achieved by burning the rest of the materials, resulting in low overall recovery levels and additional emissions.

End of life treatment case study: composite hydrogen tanks

The use of composite pressure vessels for alternative “second life” applications has had limited exploration. Development of protocols to certify pressure vessels for lower pressure applications at the end of their first life, will extend the useable life of these vessels. Research into design for end of life and composite materials reuse and recycling will also be critical in reducing their carbon footprint and moving towards a circular economy.

Developing applications for the second life of equipment, and certification standards to ensure materials are safe to be used in these applications will be beneficial to reducing their overall emissions footprint. New methods of recovering materials and reusing products at the end of their useful life will allow hydrogen energy systems to be integrated as part of a truly sustainable system.

Developing UK capability to test, set standards, and accredit new materials

Early-stage materials testing for some hydrogen applications has resulted in test methodologies that vary widely between researchers, such as those used for testing the impact of hydrogen on pipeline materials. This leads to challenges in comparing data sets and understanding the applicability of experimental results. Further, standardised safety inspection protocols are required to provide assurance of the lifetime of materials used with hydrogen, such as gas grid compressors.

Developing standardised materials testing methodologies for hydrogen will increase confidence in results and collaboration between those undertaking research in the hydrogen space, and further cement the UK's position as a leader in this field.

New standardised safety inspection protocols will need to be developed that are compatible with materials used with hydrogen. Since degradation mechanisms of materials subjected to hydrogen exposure are not always understood, it is not clear whether existing inspection and testing protocols provide sufficient safety assurance. These protocols are required to ensure safe operation of hydrogen equipment over its lifetime.

Materials inspection case study: hydrogen compressors

Since the degradation mechanisms for materials used with hydrogen at high temperatures and under high mechanical stress are poorly understood, it is challenging to identify the signs of degradation that may lead to failure of components. One example of this is gas grid compressors, where failure of components could have significant consequences for the gas grid operation and approvals. New protocols are required to provide assurance of component lifetime during a gas grid compressor inspection.

Often, materials used with hydrogen are used under extreme temperatures – cryogenic for liquid or materials-based storage, and high temperatures in heat and power applications. A wide range of pH conditions are also used, along with water (either used to produce hydrogen or produced when hydrogen is used) which can cause corrosion issues. Work will need to be undertaken to understand in-use materials degradation with hydrogen in extreme temperatures and chemical environments.

The UK has the capability to establish testing capabilities in hydrogen materials development. This will enable companies to test products here rather than seek testing capability overseas as they currently do and will serve to further underpin the UK's leadership position in this field.

Computational design of materials

Computational design and machine learning enables identification of desirable materials properties and integration of these properties into the resulting candidate materials.

The UK has leading expertise in this field. By adopting these approaches materials can then be selected and partially screened "*in silico*" prior to physical testing enabling accelerated materials development and access to a range of new insights into materials properties.

Computational design case study: Computational methods are increasingly used including robotics in a connected platform to enable accelerated discovery and development of materials which are critical to a wide range of energy applications. Examples of some of the groups active in this field include the MIF at Liverpool, Digifab at ICL, A3MD at the University of Toronto, STFC Hartree and IBM. Through a KCMC partnership, University of Liverpool and the STFC Hartree Centre are working on the integration of computation and experiment, to accelerate materials discovery with an industrial partner.

7. Conclusions and Next Steps

There is growing evidence that the hydrogen energy sector is set to become a multi-billion-dollar industry in the near future [2] [6] [30]. The UK is at the forefront in several areas of this fast-evolving sector, with advanced plans for gigawatt scale low carbon hydrogen production in industrial clusters, a well-developed programme to investigate the feasibility of converting natural gas networks to hydrogen, trials for fleets of hydrogen-fuelled cars, buses, and vans, and further innovative projects across the sector.

This Royce study set out to examine the critical materials research challenges for the hydrogen energy sector with a scope covering production, storage, distribution, and end use. The study has identified a set of five key priorities for materials research along with a sub-set of enabling areas critical to supporting materials development, uptake and use. Addressing these materials challenges underpins the UK's wider hydrogen energy sector leadership ambitions by providing potential materials solutions that can support its accelerated deployment.

The findings of this study, reached in consultation with a broad range of leading academic and industry experts, sets the immediate direction for investment of UK resources in materials research for the hydrogen energy sector. This report represents a critical first step in identifying the materials research priorities for the hydrogen energy sector. It also identifies a range of technology areas beyond the five key priorities which merit further detailed review to identify any potential future game-changers. The report aims to catalyse further collaborations between academia and industry to develop solutions in this space.

The next stage, following this report, will be to work with the contributors to this report – and other interested stakeholders – to assess the resources, funding, and partnerships required to support materials research in these key areas with a view to accelerating the uptake of hydrogen technologies in the UK.

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Appendix I – Further research topics considered

The topics in this Appendix were raised in the workshops but did not meet the selection criteria to be included in the main body of the report. It is important to recognise that this is not an exhaustive list of all potential areas of hydrogen materials related research.

Hydrogen production

- Electrolyser frame materials to reduce frame mass and cost
- Regeneration and end of life recovery for electrolysers
- Improved catalysts for steam methane reforming
- Catalysts for chemical looping and low temperature pyrolysis
- Hydrogen thermolysis from nuclear power

Hydrogen storage and distribution

- Improved gaseous hydrogen cylinders for trailer transport
- Electrochemical compression
- Catalysts for hydrogen uptake and release from LOHCs

Hydrogen use in transport

- Materials for the detection of impurities in hydrogen
- Materials for ammonia combustion in transport

Hydrogen use in heating and power

- Materials for gas metering

Appendix II – Sustainable chemistry

This section has been produced by the KTN. It summarises a report delivered by Enabled Future Limited and sponsored by Innovate UK. For further information and detail please see UK Catalysis Market Study Summary prepared for KTN/Innovate UK, Enabled Future Limited, Dr M Lynch, June 2020 and UK Net Zero carbon reduction in the areas of catalysis innovation prepared for Innovate UK, Enabled Future Limited, Dr M Lynch, Sept 2020.

A hydrogen economy will enable a wide range of sustainable chemistry pathways that could allow for the de-fossilisation of the chemical and material sectors via the production of platform chemicals. There are multiple sustainable chemical pathways to produce low carbon chemicals including CCUS pathways for which hydrogen will be a key enabler. For instance, CO_2 can be converted into CO and water into hydrogen. The conversion pathways include electrolysis, photocatalysis and other related high-energy reactions. These would replace older chemistries for converting fossil fuels such as steam reforming and gasification and even though the benefits of blue hydrogen are clear; it will require a vast amount of carbon to be sequestered and necessitate the extraction of fresh fossil fuel which creates both CO_2 and methane emissions during exploration, production and transport and results in loss of biodiversity. Diversion of carbon back into the system for utilisation would be vastly more beneficial for the environment. Hence green hydrogen via water electrolysis is one of the single most important future transformations in the chemicals industry, underpinning a whole host of downstream Power-to-X (P2X) value chains. These span larger bulk chemicals and so-called “e-fuels” including ammonia, methanol, ethanol and synthetic liquid transportation fuels.

Carbon capture utilisation and storage (CCUS) incorporating both CCS and CCU is one of the main methodologies which will be used to achieve UK NetZero. These approaches are necessary for hard-to-abate sectors where decarbonisation cannot be achieved via 100% electrification e.g. for aviation fuel, home heating and a range of other transportation modes. Carbon capture and utilisation (CCU) can be applied to production of a wide range of chemicals and fuels however it is not viable without access to low cost, low carbon hydrogen. CCUS is seen as a nearer term strategy for decarbonisation in the UK compared with Power-To-X (where X is a base chemical in the global chemical supply chains).

In future Power-to-X may be employed to dissociate nitrogen for low carbon ammonia, replacing the existing Haber-Bosch process which has a very high carbon footprint. There is also potential for high atom efficiency[3] transformations on a range of other molecules as more experience is gained. However, this is only likely to be achieved if a range of efficient Power-to-X catalysts and processes are developed. It is important that strategies and funding are provided now to ensure that there are technologies available within the next decade. Power to X where X is either methanol, ethanol or liquid fuels will support the de-fossilisation of multiple sectors including fuels and chemicals, hydrogen will again be a critical enabler for this.

Power-to-methanol refers to the conversion of green hydrogen and waste carbon dioxide into methanol. This is one of the most common types of power-To-X projects, it also opens the ability to produce green dimethyl ether (DME) and gasoline using existing technologies. As with methanol, ethanol can also be derived from CO_2 and hydrogen which would avoid many of the issues associated with current bioethanol production including product consistency from different feedstocks, competition with food crops, ground level ozone pollution, use of fertiliser and associated N_2O emissions, soil acidification, land eutrophication and others. Ethanol is a widely used biofuel manufactured by fermentation of food crops. It is commonly blended into gasoline fuel at levels of 5-10% (E5, E10) or even higher. Power-To-Liquids (PtL) generally refers to the conversion of CO_2 to any transportation fuel that can be liquefied including methanol, ethanol, DME, OME or Fischer-Tropsch (F-T) liquids. It is anticipated the electron efficient catalysts will play a key enabling role in bringing this technology to the marketplace.

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[3] Atom efficiency = molar mass of intended product ÷ sum of the molar masses of all products

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This report forms part of a suite of complementary road mapping and landscaping reports designed to stimulate and drive new advanced materials research in the UK:

- Materials 4.0: Digitally-enabled materials discovery and manufacturing
- Materials for Fusion Power
- Materials for End-to-End Hydrogen
- Degradation in Structural Materials for Net-Zero

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