Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

2022 – SusHy Projects Booklet

Updated on 06/06/2022

These are the current projects available for 2022 intake, more projects will be available soon.

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# Supported nanoalloys for sustainable hydrogen production

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Project description

This project is envisaged to create a holistic approach linking together sustainable fabrication of metal containing materials for a range of applications, focussing on photocatalytic hydrogen generation considered the "oil of tomorrow". Our ambition is to dramatically reduce the dependency on rare metals in hydrogen technology, either by replacing them with more abundant elements (e.g. Pt for Ni) or by reducing their use to the absolute minimum required, through the innovation in the science of metal nanoalloys (MNA). To achieve this transformative change, we will open up new areas of science by (i) providing scalable routes to MNA fabrication with atomically precise structure and composition using the magnetron sputtering facilities in Nottingham (ii) investigating the optical and electronic properties of the materials produced under *in situ* conditions (light and water vapour) via Near-Ambient XPS (iii) harnessing functional properties of MNC in the photocatalytic production of hydrogen using sunlight.
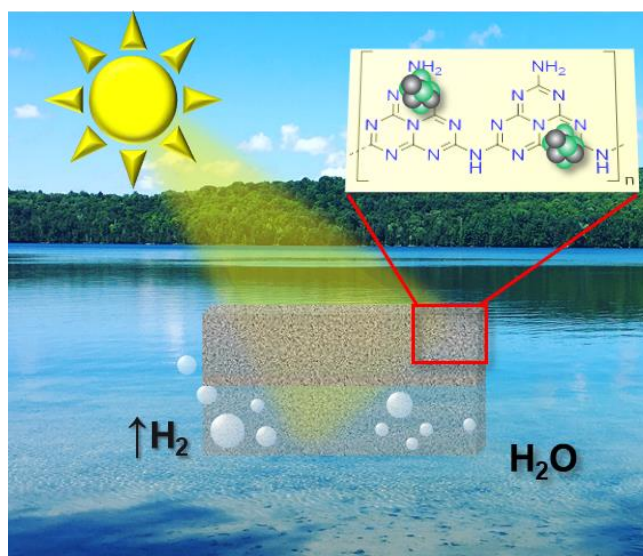
Deliverables

- Fabrication of novel heterogeneous photocatalysts based on supported MNAs with atomically precise size and composition (*e.g.,* Pt & Ni, Co, or Cu bimetallic nanoalloys).
- Atomic-level understanding of the MNA surface dynamics under *ex-situ* and *in-situ* conditions.
- Highly efficient materials for photocatalytic hydrogen production with potential to attract industry attention (e.g., JM) as materials synthesis is easy to scale up.

Investigating the use of alternative fuel pumps designs for cleaner aviation

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Project description

With the continuing drive towards cleaner aviation in recent years, there have been active investigations into alternatives to traditional aviation fuel. Liquid hydrogen is one of the leading candidates as identified by a recent (March 2022) report from the Aerospace Technologies. Fuel pumps have traditionally used fuel-lubricated bearings including plain bearings and rolling-element bearings. These bearings face very specific challenges with liquid hydrogen due to the very low temperatures, low viscosity, low density, the tendency to cause brittleness of the bearing materials and the possible chemical effects that might exist.

This PhD project sets out to investigate the selection and engineering design of bearings suitable for use in liquid hydrogen pumps. Such pumps have been used in rockets for decades but the rocket applications require an active service life measured only in minutes. This work will explore both the customisation of conventional bearing designs and the development of novel bearing designs suitable for service within a fuel pump that could operate at the required loads and rotational speeds whilst also having a long operational life spaces (>10,000 hours). It is expected that the study will embrace traditional fluid bearing designs (including plain journal bearings) as well as (electro-)magnetic bearings and it may also consider the possible exploitation of controllable unbalanced magnetic pull within an electrical machine to assist in managing bearing transverse loads.

Stakeholder collaboration: Rolls-Royce PLC

Deliverables

- Insight into the critical issues effect design and selection of LH2 for use in civil aviation.

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Innovative materials for thermal compression – Solving the challenge of hydrogen compression

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Project description

Critical to reducing UK carbon emissions is the development of efficient hydrogen storage and distribution technologies. Hydrogen gas can be compressed using innovative compression technologies but there remains significant challenges to their successful deployment. Solving the challenges of solid-state compression will have a significant impact on the delivery of compressed hydrogen for a wide variety of applications. The current Hydrogen refuelling technology exists and relies on mechanical compressors to reach 850 bar to supply 700 bar refuelling stations. Hydrogen is a light and difficult to compress gas. Typically compressing hydrogen mechanically requires an additional (ca. 20%) of the calorific value of the gas. The mechanical compressors are costly, difficult to maintain, noisy and have reliability problems especially if used intermittently.

Using the thermodynamics of metal hydrides to our advantage we can compress hydrogen gas just by heating the metal hydride store up to 150 °C. The solid-state compression of hydrogen offers a more economical alternative to mechanical compression with a higher level of safety, quiet and significantly lower maintenance regime. We are looking for researchers that are interested in discovering, and characterising new materials that meet the demanding requirements of a solid-state compressor with no moving parts. There will be significant materials characterisation of new alloys they synthesis including hydrogen uptake and release thermodynamics and kinetic measurements.

A prototype solid-state compressor has been built as part of an EPSRC funded project. The next stage, which is the purpose of the project, is to develop bespoke alloys to boost the compression range, extend their capacity, increase the kinetics and develop a state-of-the-art two stage hydrogen compressor. There will be strong industrial engagement through contact with commercial metal alloy producers and potential end users of the technology. The project will feed into a collaborative multimillion research project, *Ocean-REFuel,* led by the University of Strathclyde.
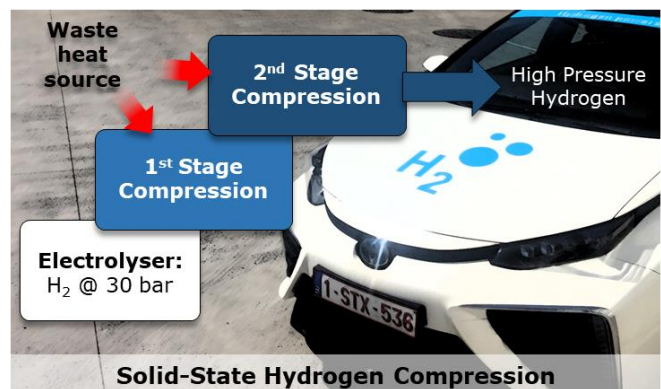
Deliverables

- Develop, full characterise and test new pairs of high-pressure alloys with flat pressure plateaus and fast kinetics to improve efficiency
- Performance evaluation of existing solid state compressor prototype.
- Design modifications to prototype system to enable it to meet and new requirements of the target operating scenario requirements.

Nanostructured hydrogen storage materials for offshore green hydrogen

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Project description

Hydrogen offers an excellent energy storage solution for the rapidly expanding offshore renewables sector. Storing hydrogen in metal hydrides is a more compact storage medium than either compressed gas or liquid hydrogen and will greatly simplify the hydrogen plant needed on an offshore hydrogen generation platform. The material challenges are to increase the capacity of the alloys and to make the metal hydride more tolerant to potential impurities from the electrolysis of seawater.

This PhD project is part of a major UK collaboration and will be working closely with our electrolyser partner at Newcastle University. Our partner will be advising on the impurities that a hydrogen store may experience. This PhD project will be investigating novel methods to improve the tolerance of metal hydrides to these impurities as well as increasing storage capacities. The research will investigate coatings, nano-encapsulation, and chemical modification to improve the hydride materials.

The successful candidate will work within a vibrant multidisciplinary research group, where we have expertise covering the discovery of new materials through to the design and application of metal hydride stores. The project will use a variety of material synthesis techniques to produce new metal hydrides, top-down and bottom-up nanostructuring, materials characterisation and hydrogen storage performance testing.

In addition to presenting work at international conferences, the project will involve research visits to our Newcastle partner and visits to the industrial partners.
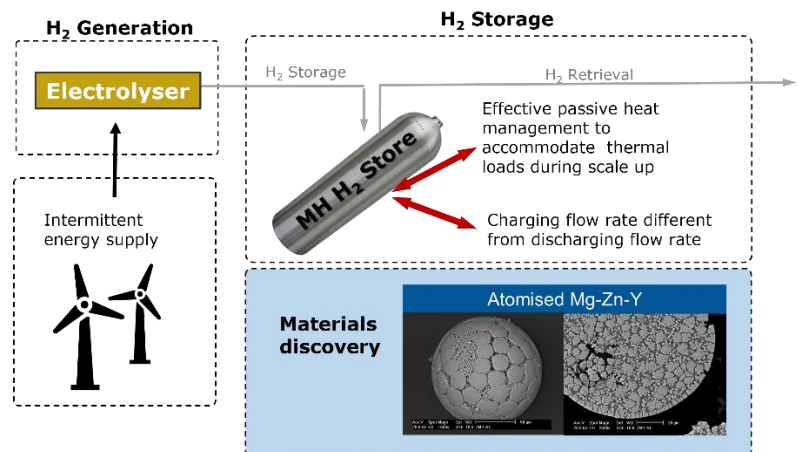
Deliverables
- Discovery of higher capacity metal hydrides.
- A fundamental understanding of the most effective chemical and structural means for impurity tolerant metal hydride stores.
- Design and experimentally prove optimised bed formulations.

# Bioinspired catalysts for green hydrogen production technologies: natural and artificial metalloenzymes

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Project description

Nature is highly efficient at producing and utilizing hydrogen. In this project we will learn from the natural catalysts for hydrogen reactions, the hydrogenase enzymes, in order to design robust and sustainable bioelectrocatalysts for green hydrogen production. While hydrogen technologies are fast-approaching everyday life, it becomes crucially important to ensure that these are fully sustainable. Full implementation of "green hydrogen" (*i.e.* H_2 generated from renewable resources rather than fossil fuels) requires the availability of clean catalysts that can easily reduce protons from water into molecular hydrogen. Water electrolysers rely on rare noble metals, such as platinum and palladium, that are unsuitable for large scale operations for both economic and sustainability reasons. In nature, hydrogenase enzymes rely exclusively on cheap and abundant metals (iron and nickel) to produce hydrogen at high efficiency and extremely fast turnover rates. Unlike synthetic chemo-catalysts, enzymes can be produced entirely from renewable feedstocks and have a very low metal requirement. Previous studies have shown that hydrogenases can be embedded in artificial devices and can effectively produce hydrogen. However, the performance over time is low, due to inherent protein instability. This project will develop novel artificial metalloenzymes (ArM) with improved stability, to be integrated into hydrogen evolution devices. In the first phase of the project, small and robust proteins will be used as scaffolds to build bimetallic clusters (either FeFe or NiFe) that mimic those found in natural enzymes. The electrocatalytic features of these artificial enzymes will be tuned by modifying the local environment hosting the metal cluster by either protein engineering (first and second coordination sphere) and organometallic synthetic methods (non-protein ligands). In the second phase of the project, the artificial metalloenzymes will be tested for electrocatalytic H_2 production and compared with existing oxygen-tolerant natural hydrogenases available in our laboratory. Both natural and artificial enzymes will be immobilised on electrodes and the hydrogen evolution reaction (HER) will be characterised under standard conditions. In collaboration with our partners at QUB, the electrodes will be modified by applying bespoke conductive gels that will protect the enzymes and further improve stability. This will enable thin layers of bioelectrocatalyst to be coated on electrodes, whilst providing an engineered environment to protect the protein. Ionic liquids will be studied as electrically conducting co-dopants that have a proven track-record of protein stabilisation.
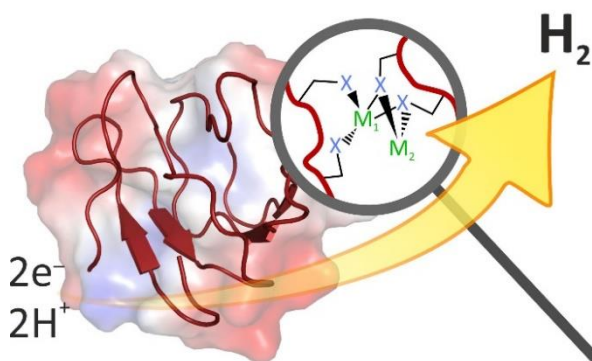
Deliverables

- Novel enzymatic catalysts for hydrogen generation based on earth abundant (Fe Ni) centres.
- Fabrication and validation of gel-protected electrodes for bioelectrochemical exploitation of hydrogenases

# Highly efficient molecular hydroge-evolution catalysts

Graham Newton and Lee Johnson

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Project description

Molecular hydrogen evolution electrocatalysts allow the efficient production of hydrogen from water under mild conditions. We will develop fully tailorable molecular clusters based on molybdenum/tungsten and sulfur/oxygen. The systems will be combined with conductive nanocarbon materials to develop highly efficient composite electrocatalysts for the water splitting reaction. We will explore the stability and efficiency these systems during prolonged electrolysis.

Conductive Nanocarbon Support
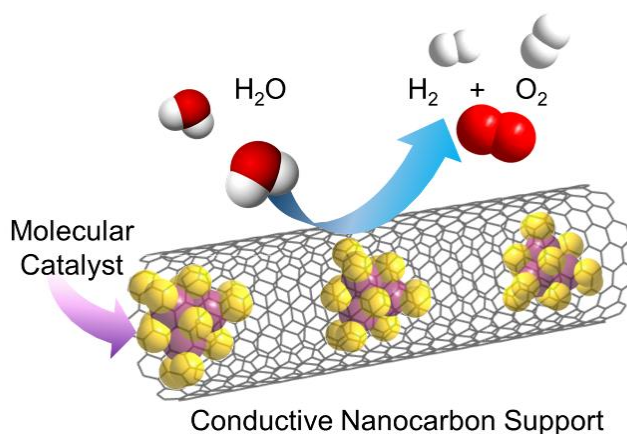
Deliverables

- We expect to design a new generation of inexpensive electrocatalysts that could outperform the state-of-the-art materials, while allowing atomic control of catalyst structure. The cheap and easy-to-prepare systems are particularly interesting from a commercialisation perspective given the ease with which their preparation can be scaled-up.

Water splitting beyond the volcano plot

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Project description

Advances and understand of electrocatalysis have reaped significant improvement in the performance of fuel cell catalysts. While similar improvements in understanding have been achieved in water splitting, this has not translated to enhancement in electrocatalysis of these reactions. Primarily, this is due to the instability of bulk oxygen evolution catalysts at higher anodic potentials, under which metal leaching and performance fading is common, and common volcano relationship due to intermediated binding. However, they these limitations are NOT inevitable. Here we propose to build on our expertise in non-aqueous oxygen electrochemistry to develop new theory and catalysts for water splitting. Leaching of active metal sites occurs because multivalent metal oxides are partially soluble (and thus corrode) in aqueous environments, but a transition to non-aqueous/water mixtures would drastically alter the solvation chemistry and thus the performance and stability of the catalyst. Our recent work has revealed the principles that control protic aqueous reactions in water water/organic mixtures, and this will provide the foundation from which we will optimise catalytic performance. Unlike catalysis in aqueous environments, which rely solely on surface adsorption at active sites, we will tune reaction profiles by solvation (due to the rich solution chemistry available in water/organic mixtures). Working with two activity descriptors will allow us to overcome the hard thermodynamic limits (volcano relationships) found in conventional water splitting. Concurrently, these systems will be designed to reject multivalent ion solvation which will enhance catalyst stability and lifetime.
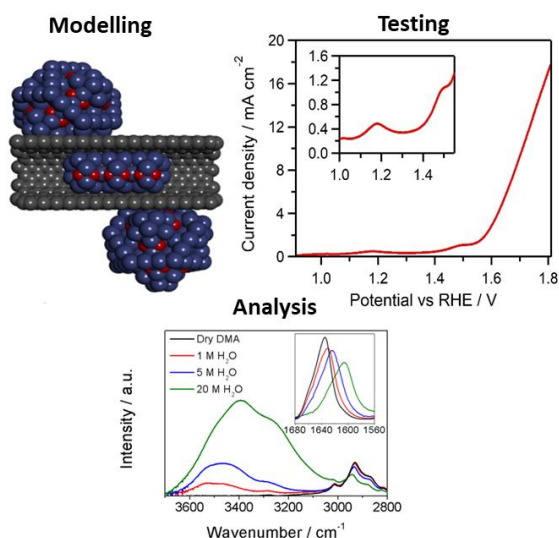
Deliverables
- New models that extend electrocatalytic theory to aprotic liquids.
- Electrolyte/catalysis combinations that offer improved stability and long-term performance for H_2O electrolysis compared to conventional aqueous based systems.
- First prototype demonstration.

H2COOL - dual energy store for refrigerated transportation

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Project description

This research is part of H2COOL, a University of Nottingham £1m research project, with the aim to produce an innovative and cost-effective dual-use energy storage technology. The dual-use hydrogen store is an integrated hydrogen technology, which will simultaneously provide the controlled release of hydrogen for a fuel cell and cooling for refrigeration. An important target application for the dual-use store are hydrogen fuel cell heavy goods vehicles transporting perishable goods i.e. refrigerated HGV's. Conventionally, hydrogen is stored at high pressure typically 35 MPa (350 bar) or greater but storing hydrogen using metal hydrides alloys offers some significant advantages. These include a higher round trip efficiency and a higher level of safety. In addition to these advantages, the dual-use energy store utilises the endothermic dehydrogenation of a metal hydride to generate useful cooling, whilst also supplying hydrogen to a fuel cell.

The success of the H2COOL project relies on the formulation and validation of new metal hydrides suitable for use in the dual-use store. The PhD student will work within a creative multidisciplinary team. This PhD project is focussed on the synthesis and characterisation of novel metal hydrides and will be working alongside scientists using materials modelling for the discovery of new formulations, engineers investigating the design of a dual-use energy store and business sociologists investigating barriers to the market. This PhD will suit candidates who are enthusiastic about applied theory and experimentation. An interest in material science and sustainable energy technologies would be beneficial. There will be opportunity for industrial engagement with both UK and international companies from the cold economy. There is also the potential opportunity for a secondment through collaboration activities with Sandia National Laboratories based in the US.

New metal hydride making and testing

Material synthesis | Characterisation | Application: Refrigerated
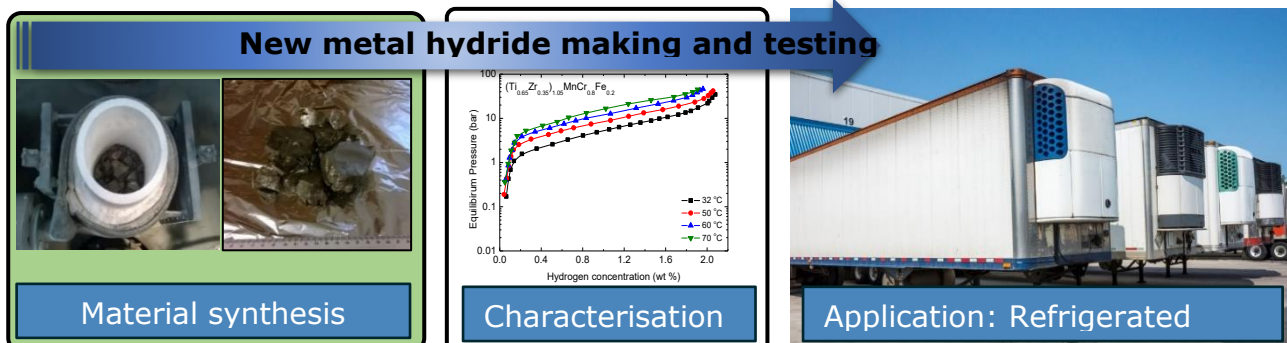
Deliverables
- New family of higher capacity metal hydrides with suitable thermodynamic characteristics to provide cooling for refrigeration.
- Proven formulation of intermetallic alloy suitable for use in dual-use metal hydride store.

Sustainable catalysts for low temperature and pressure ammonia synthesis

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Project description

There is a lot of interest in using ammonia as a hydrogen rich energy vector, not just for the more efficient moving of energy to different markets, but also direct combustion of ammonia as a fuel to help decarbonise heavy vehicles such as for road freight, rail and marine sectors. Ammonia is produced industrially through the Haber Bosch process, but needs high temperatures (300 - 450°C) and high pressures (150 – 200 bar). Unfortunately, this makes the process unsuitable for smaller scale intermittent generation of ammonia for example distributed generation coupled with either wind or solar renewable energy. A more agile ammonia synthesis requires a catalyst that can operate at lower temperatures and lower pressures.

Currently ruthenium is the only catalyst that has acceptable kinetics at low temperatures. This project will investigate more sustainable catalysts that avoids the use of resource limited platinum group metals. The novel catalyst design will utilise transition metal alloys, supported on metal hydrides. The metal hydride will act as a hydrogen pump, supplying hydrogen to the catalyst enabling rapid hydrogenation of the adsorbed nitrogen. Catalyst will be deposited onto metal hydride supports using magnetron sputtering to control the catalyst coverage, but also to investigate compositional change of the deposited catalyst through graded deposition.


To produce several test transition metal alloys that dissociate nitrogen effectively (i.e., substitute to Ruthenium) and successfully magnetron sputter (PVD) coat onto an effective hydride support, which dissociates the hydrogen efficiently. Catalyst activity will be compared with the material characteristics in order to optimise the design of the catalyst and hydride support.
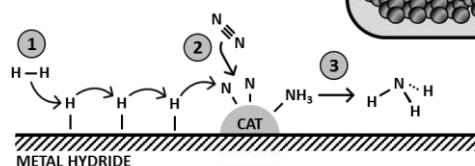
Deliverables

- Identified transition metal catalysts with comparable activity to ruthenium.
- Optimised catalyst coating onto metal hydride particulates.
- Maximise the synergistic effect between the catalyst and metal hydride support.
- Experimentally validate the catalyst efficacy during intermittent operation.
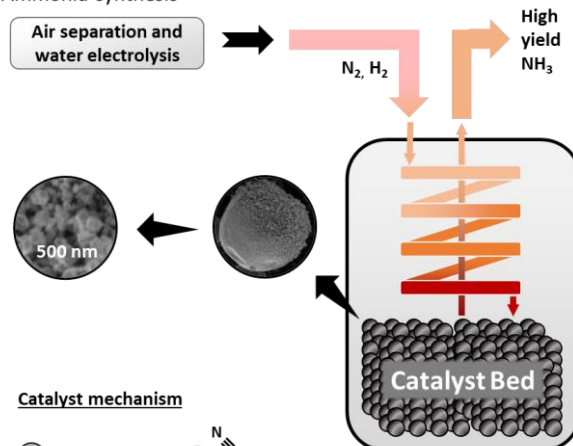
Decarbonised Clean Heavy Duty Engines via Hydrogen and Ammonia Flex Fuelling

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Project description

This experimental research will directly compare two new promising retrofit viable combustion systems capable of converting existing diesel engines for fully flexible hydrogen or ammonia fuelling. The first solution is shorter term and based upon dual fuel (small biodiesel pilot in to ammonia and/or hydrogen main fuelling). The second system eliminates the pilot fuel entirely and involves adopting a novel turbulent jet ignition system currently used in Formula 1 to speed up combustion and to be used here to improve NH_3 and H_2 combustion for ultra low NOx. The goal is to improve fundamental understanding and accelerate this promising Net Zero compliant technology to market with the key UK supply chain engaged.

UoN Heavy Duty Dual Fuel Research Engine
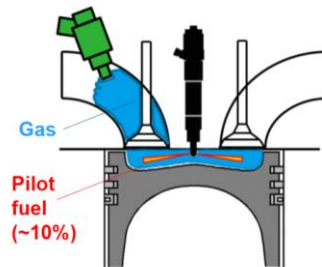
Compression Ignited Dual Fuel
- Port fuel injection of NH_3
- Pilot injection (e.g. diesel)
- Lean burn (high efficiency)

Deliverables
- Fuel injection characterisation in a new optically accessed "bomb" being commissioned within the RAD building at UoN, with data being used to develop new CFD models of NH_3/H_2 injection
- On engine testing and operating strategy development for best trade-off between thermal efficiency and NOx

Machine Learning Discovery of Electrocatalysts for Sustainable Hydrogen Production

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Project description

Sustainable production of green hydrogen from water splitting using renewable energy sources such as wind and solar is a very promising approach for both short-term balancing and long-term inter-seasonal energy storage. Development of efficient, stable and cheap electrocatalysts is of paramount importance to large scale green hydrogen production. The chemical compositional space of electrocatalysts is too large to be explored efficiently using pure experimental approaches. Discovery of new electrocatalysts for hydrogen production can be significantly accelerated by a combination of density functional theory (DFT), machine learning (ML), and experimental approaches. It has been demonstrated that the free energy of hydrogen adsorption can be used to quantify the activities of different electrocatalysts in the hydrogen evolution reaction. In this project, we plan to perform high-throughput DFT calculations of hydrogen adsorption on carefully selected high-entropy alloys (HEAs), and we will use these data to train an accurate ML model. Our ambition is to screen the HEA compositional space *exhaustively* using the ML model, in order to identify efficient and cheap HEA electrocatalysts for green hydrogen production. Working alongside our local and international experimental collaborators, the most promising candidate HEA electrocatalysts discovered from the ML screening will be synthesised and characterised, and their activities for electrocatalytic hydrogen production will be validated by experiments.

electrocatalyst for hydrogen production
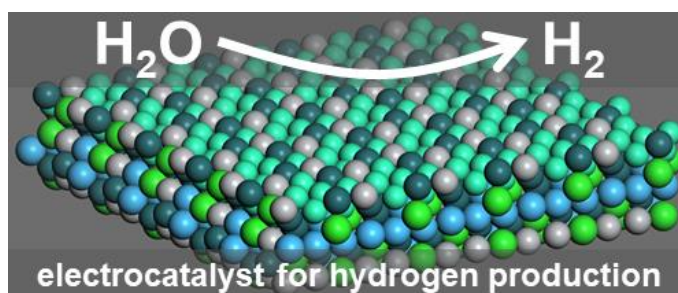
Deliverables

- Database of high entropy alloys with DFT predicted structural and thermodynamic properties on hydrogen adsorption
- Machine learning model for predicting the free energy of hydrogen adsorption on any given HEA surface

Green hydrogen production from water splitting powered by renewable electricity

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Project description

Water splitting via an electrolyser powered by renewable or excess electricity is a full solution for sustainable net-zero production of green hydrogen, however, it is an energetically uphill process involving the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode. Whilst the 2-electron HER is relatively facile, the 4-electron OER is particularly sluggish and requires noble metal (Ir, Ru) electrocatalysts under acidic conditions. However, under alkaline conditions, OER is much facile and significant progress has been made recently where non-noble metal electrocatalysts such as transition metal (Ni, Fe) based layered double hydroxides (LDHs), phosphides and nitrides were effectively used for OER, and the latter two were also proven as bifunctional electrocatalysts for HER as well for OER.

Build upon our nascent work on new electrocatalysts and electrodes for the OER anode and HER cathode, and the anion-exchange-membrane (AEM), in this project we will integrate the state-of-art electrocatalyst materials onto the alkaline AEM to develop membrane-electrode-assembly based water electrolyser, for sustainable hydrogen production with the maximum resource and energy efficiencies. We will pay particular attention to the catalytic electrode-electrolyte interface engineering to achieve efficient reaction kinetic, and fast charge and mass transports in the water electrolyser, to minimise overpotential loss and gain maximum voltage and overall system efficiency.
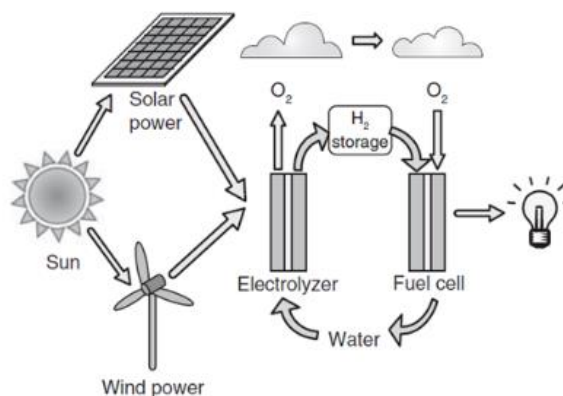
Deliverables
- A low-cost and scalable water electrolyser demonstrator for green hydrogen production, having an optimised scaffold structure and avoiding the use of noble metals, together with an in-depth understanding of the catalysis and electrochemical interactions involved.

Stakeholder Collaboration: Guangdong Longhu Sci & Tech company Ltd

Social Hydrogen: Hs

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Project description

To move to the next generation of fuel cells not only requires the science but also the acceptance and demand from customers, which is influenced by the messaging, promotion, and support of critical public and private stakeholders. To fully understand the complex landscape (political, commercial and consumer) the project will develop a system of systems of ontologies that can mine information from social media platforms, publicly available commercial documents and government web sites and policy documents to build a real-time map of the drivers, inhibitors, perceptions and consumer influencers. The real-time analysis will provide semantic models of the landscape and have various lenses that will highlight the socio-technological change required e.g. the degree of uncertainty towards technologies and their use in everyday items like vehicles. In turn, this will direct how future messaging, policy, and advertising needs to be engineered to respond to the existing 'social' landscape.

The generic system of system ontology and real-time mapping capability will be trialled using an automotive case study, evaluating the use of hydrogen for the case study's transportation fleet. Current awareness and perceptions of hydrogen fuel cells suggest that demand for vehicles is extremely low due to many misconceptions and better publicity and support of alternatives e.g. battery. Specifically, this research will aid automotive companies in developing their next generation powertrain vehicle offerings (core and augmented), which will inform and aid the supply chain. It will also provide government with insights into the blockers and how they can enable a quicker route to net zero across the population. This project will take elements of an existing digital tool, EMOTIVE (developed and owned by the research team). However, a new architecture will need to be researched and developed for this proposed work including the system of systems ontologies. A new Hydrogen Natural Language Pipeline with semantic technologies will be developed within the system of systems framework.

The Team are well placed to deliver this project as they hold extensive experience in EMOTIVE technologies and years of experience in the hydrogen domain, as evidenced by the latest funded project *Robust Lifecycle Design and Health Monitoring for Fuel-Cell Extended Performance (RESILIENCE)* – (Supergen EPSRC EP/K02101X/1).
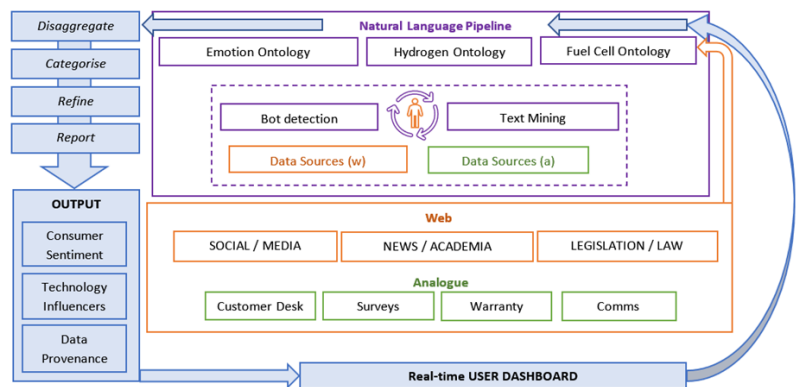
Deliverables

- Sematic ontology of the hydrogen fuel domain
- Interrogatable semantic system to determine enablers, inhibitors/blockers, and key influencers
- Commercial facing dashboard for data segmentation and analysis
- Foundation for an automated digital text-mining interface.
- Interface for collaborators to interrogate the social map to aid decision making

Understanding the lifecycle carbon footprint and costs of sustainable hydrogen energy systems

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Project description

Hydrogen is considered as a clean fuel for the future. Yet it is important to recognize that its production, distribution, and usage may have negative impacts on the environment, society, and the affordability. Examining the carbon footprint, energy requirements, costs and social impacts from a life cycle viewpoint of different hydrogen technology routes (e.g., green turquoise or blue hydrogen) will form a complete picture of the sustainability of the future hydrogen technology options.

Here the research challenge is to gain insights into the whole energy and industrial system around the new hydrogen production and application routes over the entire lifecycle, instead of just looking at single point. Sustainability may only be assessed by means of a systems-wide approach, which combines economic, environmental, and social impact indicators. This project will combine system integration (SI), technoeconomic and lifecycle assessments (TEA & LCA) and multi-criteria decision making (MCDA) framework as essential tools, to enable such industrial symbiosis innovation, by systemic assessing hot spots of carbon footprint and their associated economic, environmental, and social impacts, and identifying opportunities for improvement at the whole industrial system level. We will integrate the aforementioned suite of whole system tools, and link them with a process digital twins to create a real-time assessment platform for the wider hydrogen systems. The innovative aspect is the proposed digital-twin informed MCDA framework embracing the SI, TEA, LCA and social impact data, allowing real time reflection of impacts with changing processes and technologies, and thus, enabling advisory features for sustainability-aware decision making during the early stage of sustainable hydrogen technology development.

Deliverables

- A novel methodology and framework that can systemically assess the life cycle carbon footprint, and their associated life cycle cost and environmental impact for novel hydrogen systems, infrastructures, and integrations; compared to the state-of-the art technology evaluations in the UK, Asia and global context.

Stakeholder Collaboration: Guangdong Longhu Sci & Tech company Ltd

Investigating the economic value of nuclear-hydrogen

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Project description

As the generation mix in energy systems is characterised by an increasing penetration of generation from renewable energy sources (RES) energy imbalances are becoming more prevalent and potentially more costly to mitigate in the absence of flexible and cost-effective forms of storage. Natural gas and other fossil fuels have traditionally provided the necessary level of flexibility over different timescales (overnight to seasonal) to the system even as the system has become increasingly subject to the variability of generation from RES. However, the pursuit of Net Zero objectives requires a reduction in the use of natural gas and the need to consider other technologies or mechanisms that can guarantee the resilience and flexibility required to underpin the effective operation of Britain's energy system.

In order to address these technological and economic challenges the project will build from an existing time-series comparison model which calculates energy imbalances in the GB system under a range of scenarios and considers the role and characteristics of various conditions required to mitigate these imbalances, e.g., the level of overnight storage required. This model was developed by the Energy Informatics Group at the University of Birmingham and will be suitable to be extended to include additional electrical generation technologies (in addition to wind, solar and nuclear) and potential storage technologies including hydrogen and interconnectors. Economic modelling will also be used in order to assess the value provided by the different generation and storage technologies to the system and the wider costs associated with different types of generation mixes able to address the simulated system imbalances at different time horizons (short term, seasonal and long term). The economic analysis will also involve an evaluation of the net present value (NPV) of investment required for different technological options.
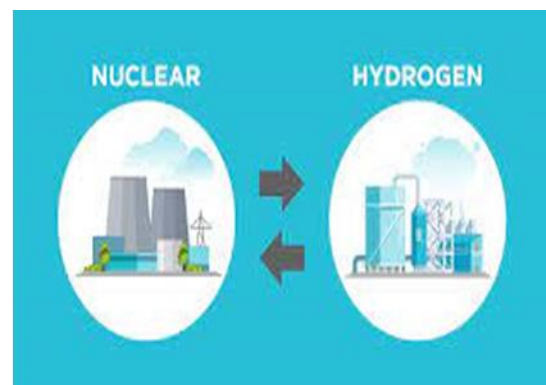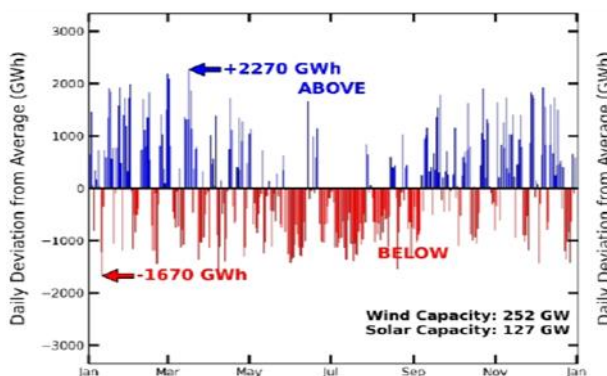
In this project nuclear power will be considered as a potential source of both power and flexibility. The reasons for considering nuclear with hydrogen as a possible alternative to natural gas are numerous. These include nuclear power's lower associated CO_2 emissions and its ability to generate predictable

amount of power (unlike RES), albeit in a less flexible way than with natural gas. Furthermore, the consideration of nuclear power and its interface with the hydrogen economy will allow for the possibility to store baseload power when not needed by the system or, for example, to be used for seasonal heating via injection into the gas network and storage over seasonal timeframes, increasing the flexibility options for this fuel. Thus, this project's potential domain extends to consideration of balancing not only within the electricity system, but across an emergent net zero energy system. As such, the project would potentially consider how conversion of nuclear based electricity into hydrogen not only provides storage and balancing opportunities but may also increase the return to and value of nuclear investments, by providing alternative vectors for storing and consuming energy derived from nuclear power. In essence, the project will explore the role, costs and potential value of nuclear to the wider energy system in its transition to net-zero and beyond.

Deliverables
- A tool for assessing economic costs and benefits of nuclear power with hydrogen to the GB energy system
- A model of energy imbalances in the GB energy system which includes nuclear plants with access to hydrogen conversion facilities

Stakeholder collaboration: National Nuclear Laboratory

Metal membranes for separating pure hydrogen from gas grids

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Project description

Hydrogen is widely regarded as a promising alternative to carbon-based fuels. However, developing hydrogen as a major energy carrier, will require solutions to many technological challenges, such as how to economically provide ultra-pure hydrogen for use with PEM-FC applications.

Hydrogen produced from natural gas reformers and from biomass sources, usually contains small amount of impurity gases, such as carbon monoxide, methane, and sulphur. Also, if hydrogen is distributed via pipelines, it tends to pick up various impurities. A PEM Fuel Cell (PEM-FC) converts hydrogen and oxygen gases into electricity; however, even very small amounts of impurities in the hydrogen can reduce the operating life of the PEM-FC.

Metallic diffusion membranes can be used to purify hydrogen. When certain Pd-based alloy foils are heated to about 300 °C, they will only allow hydrogen gas to pass through, resulting in parts-per-billion level pure hydrogen. However, the conventional Pd-Ag membrane alloy used is extremely expensive, and there are not able to tolerate certain impurities (i.e. they can be poisoned).

This project will investigate Pd-based alloys, which contain: (1) much lower amounts of Pd, which theoretical studies have suggested should have good hydrogen permeability values; and (2) additions that change the surface chemistry of the alloys (i.e. could make them more resistant to poisoning).
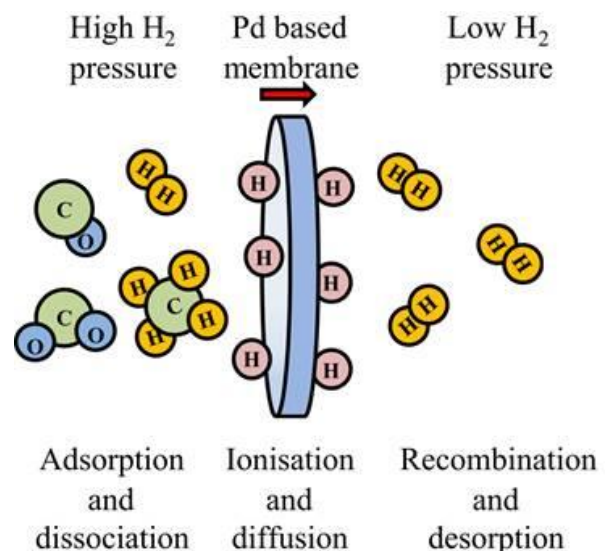
Deliverables

- Pd alloy foils and/or supported films with improved resilience to: (i) natural gas; and (ii) impurities and odorants likely to be found in converted hydrogen gas pipelines
- Lower cost Pd alloy membranes, via changes in composition and processing
- Design of system for Metal Membrane gas separation for integration with gas pipelines (CH_4/H_2 and H_2 grids)

# Modified transition metal catalysts for hydrogen and oxygen evolution

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Project description

Transition metal dichalcogenides (TMDs, eg MoS_2, WS_2) have been the subject of intense research in recent years as low-cost catalysts for H2/O2 evolution. The chemistry of the catalytically active sites is currently becoming more understood, and this project seeks to build on these recent advances through: (i) maximising edge sites through controlled TMD electrodeposition forming porous structures, (ii) modifying the catalytic sites through metal doping, (iii) optimising the stability of active sites.
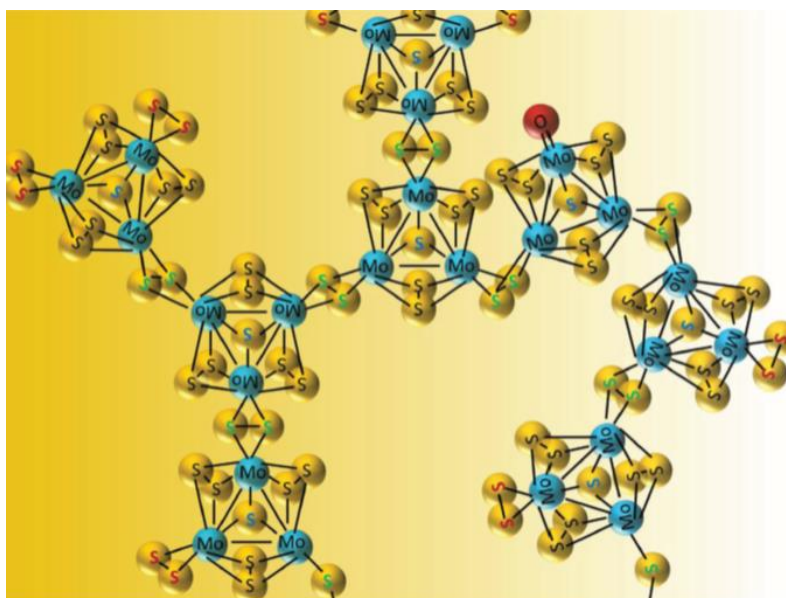
Deliverables

- Fabrication of range of layered TM compounds via different methods, with physical characterisation followed by electrochemical characterisation as catalysts for HER/ORR and other relevant reactions, and quantitative evaluation of mechanistic details

Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

Business cases for Green Hydrogen
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Project description

It is generally agreed that hydrogen employed in sustainable and emission-reducing projects needs to be sourced from 'green' feedstock and energy. Nevertheless, the vast majority of hydrogen sold today is 'black' and produced by steam reforming of natural gas. Obviously, there are issues with cost. This work will be looking into how green hydrogen can be costed so that it is better compatible with today's energy system. This includes analysing business cases, high-value applications, externalities, and options to sell 'greened' products based on green hydrogen application.
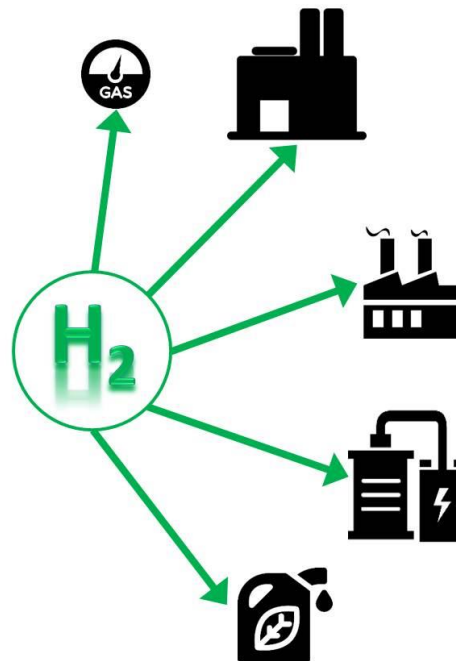
Deliverables

- Cost model fully established.
- Environmental pricing added to cost model.
- Business model development concluded.
- Dialogue with industry, validation of models and approaches

Hydrogen safety in rail applications
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Project description

The rail sector presents a particular safety challenge for hydrogen and fuel cell systems due to comparatively larger inventory, confinement of storage, high speed and vibrations, currently accepted large hydrogen flow rate from thermally activated release devices (TPRDs), passengers located in vicinity to high-pressure hydrogen storage and exposed to potential pressure and thermal effects, narrower rail tunnels cross-section profile preventing quick hydrogen dispersion below low flammability limit (and thus creating conditions for flammable envelope deflagration), etc. This PhD project will start with a review of relevant hazards, available safety strategies and engineering solutions for high-pressure hydrogen storage in rail applications. Relevant to rail accidents and the design of hydrogen-powered trains information will be critically analysed. Innovative safety strategies and engineering solutions will be proposed and corresponding incident scenarios will be simulated to demonstrate reduction of hazards and associated risks. This includes engineering solutions for TPRD and hydrogen venting lines design, etc. Fire onboard a hydrogen-fuelled train while in a tunnel presents the worst credible accident scenario. Consequences of incidents in tunnels of various shape, span and height will be investigated in terms of pressure (overpressure, impulse) and thermal (temperature, heat flux, thermal dose) effects on life and train. Particular attention will be paid to hydrogen jet flame impact on rail cars and passengers safety, and structural integrity of hydrogen storage compartments under fire conditions.

The performance of available engineering solutions, e.g. explosion free in a fire self-venting TPRD-less storage tanks, in arrangements characteristic for hydrogen trains will be studied to formulate requirements for their safe operation in normal and fire conditions.

The successful candidate will undertake this doctoral study at HySAFER Centre, one of the key providers of hydrogen safety research and education globally. S(he) will focus on theoretical and numerical modelling with the use of relevant ANSYS software and the Northern Ireland High-Performance Computing (NI-HPC) Kelvin-2 cluster. The results of this doctoral research will be used to support HySAFER's externally funded projects, reported at international conferences, and published in peer-reviewed journals.

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Deliverables

- Hazards identification and selection of incident scenarios
- Problem formulation for CFD and/or reduced engineering model simulations
- Model implementation, validation and use for hydrogen safety engineering
- Innovative safety strategies and engineering solutions for hydrogen trains

Hydrogen safety for marine vessels and port infrastructure

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Project description

Decarbonisation of transport including the maritime sector is an integral part of the UK Government "The Ten Point Plan for a Green Industrial Revolution" and "UK Hydrogen Strategy" both set plans for an accelerated transition to sustainable transport. The PhD project will review the existing knowledge on safety design and operations of hydrogen systems and infrastructure in the maritime sector.

The IGF Code (International Code of Safety for Ships Using Gases) provides the regulatory framework for the adaptation of low-flashpoint marine fuels like hydrogen. The finalization of the Fuel Cells Interim Guidelines is foreseen in 2021. No work to cover storage of hydrogen as a fuel has been initiated in IMO. According to the IGF Code Part A, a low-flashpoint fuel like hydrogen is allowed as long as the Alternative Design approach demonstrates that the hydrogen-specific systems are as safe, reliable, and dependable as new and comparable conventional oil-fuelled ships. IGF Code Part A details requirements for risk assessments and analysis of explosion consequences to ensure that the necessary assessments are carried out to eliminate or mitigate adverse effects on people on board, the environment, or the ship.

This doctoral study will close essential knowledge gaps and contribute to the IGF Code and relevant documents (IMO CCC7/3. (2020); IMO MSC.1/Circ.1455; IMO MSC.1/Circ.1212/ Rev.1) by addressing the following issues: hydrogen containment, hydrogen bunkering systems, fuel cell and power generation safety, ventilation, control and monitoring, etc. The study will formulate requirements to the ventilation system to control "standard" and unscheduled releases below the regulated level for initiation of alarm and protection system. The double-wall requirement for fuel lines will be analysed and new requirements will be formulated accounting for hydrogen properties. The engineering

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solutions to mitigate the pressure peaking phenomenon (specific only for hydrogen) will be developed. Interaction of hydrogen jet fires with vessel structure will be studied and mitigation measures suggested. Mitigation of non-uniform hydrogen deflagrations by limiting the released inventory and venting technique in vessel enclosures will be proposed, etc. Bunkering is another area where knowledge gaps to be closed, including the fuelling protocols.

The candidate will develop a structured approach to hazard identification, the definition of incident scenarios and performing hydrogen safety engineering to quantify incident consequences and estimate

associated risks. Innovative safety strategies and engineering solutions will be developed to keep the risk of hydrogen-driven marine vessels at the level of current vessels or below.

The successful candidate is expected to have a strong background in one of the following disciplines: engineering, physics, mathematics, fluid dynamics, heat and mass transfer, combustion. Any previous experience in theoretical analysis and/or numerical studies is welcome. The research will be conducted at the HySAFER Centre. The candidate will focus on CFD modelling and numerical simulations, use relevant software (ANSYS Fluent, FieldView, etc.) and the state-of-the-art computational resources – multi-processor workstations available at HySAFER Centre and Kelvin-2 High-Performance Computing facilities. This research will be aligned to relevant HySAFER's projects, results reported at international conferences and published in peer-reviewed journals.

Deliverables

- Identification of hazards for hydrogen use in marine applications;
- Analyse case studies and relevant statistics to formulate scenarios for hydrogen safety engineering of hydrogen-powered vessels;
- Develop and validate models for assessment of consequences of incidents;
- Develop safety strategies and engineering solutions for design of inherently safer marine applications.