Sustainable Hydrogen

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2022 – SusHy Projects Booklet

Updated on 08/12/2021

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

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Composite membranes for H_2 purification

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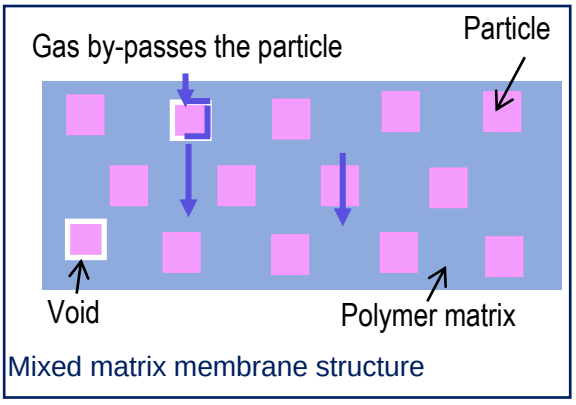
Project description

H_2 is a high quality and clean energy carrier. Currently, the majority of hydrogen is produced by steam-methane reforming followed by a water-gas shift reaction whilst bio-hydrogen production has also been increasing. Before hydrogen can be used in fuel cell and other applications CO_2 and CH_4 must be removed that resulted from production processes. Membrane-based separation technologies are one of the most promising alternatives compared to conventional separation technologies i.e. pressure swing adsorption because of low energy consumption. Although many inorganic membranes of zeolites, metal alloys and carbon molecular sieves have developed, the difficulty of scaling up limits their applications.

Polymer membranes are useful whilst controlling permeability/selectivity in harsh conditions is challenging. Recently mixed matrix membranes (MMMs), where an inorganic material embedded into polymer matrix, have attracted more attention as they combine porous materials' functionality with polymer processability. In this sense, metal–organic frameworks (MOFs) that comprised of metal ions connected by organic linkers, are the most promising ones due to their diverse and flexible structure. In addition, the organic linker in MOFs typically have better affinity towards polymer chains and thus allow control of the MOF/polymer interface. Therefore, void-free MMMs can be prepared without the requirement for modification of filler or membrane surfaces.Therefore, this project will explore development of metal organic framework/polymer mixed matrix membranes with enhanced H_2 selectivity to enable membrane-based H_2 purification.



Mixed matrix membrane structure

Deliverables

- TIFSIX/SIFSIX syntheses recipes to yield specific size and shape.
- Flat sheet film prep routes and characterisation of membranes
- H_2 purification performance of membranes manufactured via MMMs

Stakeholder Collaboration: National Grid

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Advanced Hydrogen Sensing Platform Based on Functionalized Metal-Organic Frameworks

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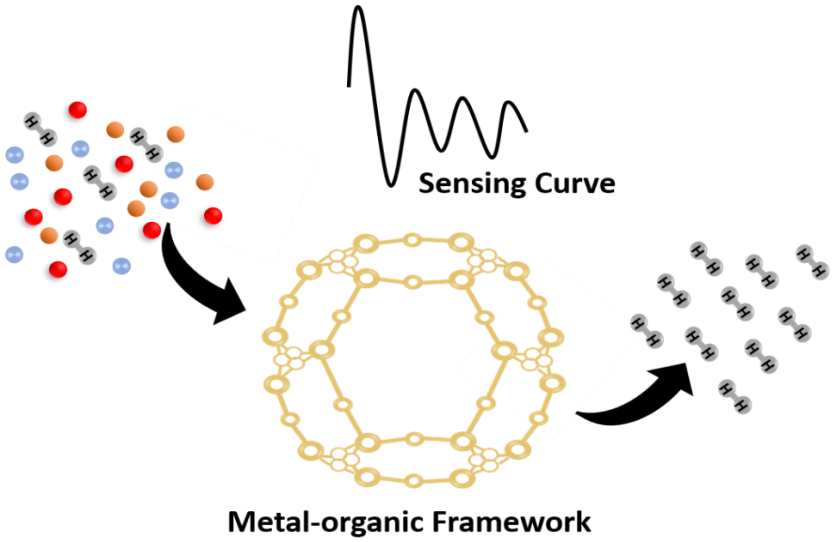
Project description

Developing efficient sensor materials with superior performance for selective, fast, and sensitive detection of hydrogen is essential for environmental protection and human health. Metal–organic frameworks (MOFs), which are crystalline and porous solid materials constructed from metal nodes (metal ions or clusters) and functional organic ligands, have received attention for gas sensing due to their large surface area, adjustable pore size, tunable functional sites and intriguing properties, such as electrical conductivity, magnetism, ferroelectricity, luminescence and chromism. However, selectivity, sensitivity and stability are still the major challenges for MOFs–based sensors used in hydrogen detection. Accordingly, this project aims to fabricate novel multifunctional MOFs with improved sensitivity and stability for hydrogen detection. The rational design of these robust, multifunctional MOFs will be guided by computational predictions in after integrating metal nodes, functional ligands, and guest molecules with different properties to achieve selective sensing of hydrogen over multiple cycles. Computational modelling will be delivered in collaboration with the Computational Materials Group at Nottingham.



Deliverables

- A library of novel, multifunctional MOFs with complete characterization data.
- Robust MOF-based hydrogen sensors capable of retaining high performance over multiple cycles.

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Base Metal Catalysis of Acceptorless Alcohol Dehydrogenation for Hydrogen Storage

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Project description

Catalytic acceptorless alcohol dehydrogenation is an atom-economical approach for alcohol oxidation without the need for an oxidant. Reversible dehydrogenation/hydrogenation catalysis from this reaction provides a route to the use of organic molecules derived from biomass as liquid organic hydrogen carriers (LOHCs). Alcohols such as ethylene glycol, glycerol and the C_4–C_6 analogues erythritol, xylitol, and sorbitol are considered to be potentially useful biomass-derived feedstocks since they can be derived from agricultural or lumber resources, including waste streams and their gravimetric hydrogen storage capacities (Figure 1) meet targets set by the EU and the US Department of Energy.

This chemistry has long been dominated by the platinum group metals (PGMs), with an elegant recent example being the report of a reversible liquid to liquid organic hydrogen carrier system using ethylene glycol and a ruthenium pincer complex. However, the low abundance of PGMs leads to high economic and environmental cost, and their high toxicity means that their removal from products often is required, producing significant waste streams. It is therefore essential that researchers look to other catalysts for industrial processes, with obvious candidates being base metals that exhibit low cost, high natural abundance, uniform global distribution and low toxicity. This project will investigate a range of low-coordinate and pincer complexes of the first-row transition metals in order to achieve the acceptorless dehydrogenation reactions, and, with appropriate candidates, investigate the possibility of undertaking the reverse reaction with addition of H_2. The first- row transition metals, with their low metal-ligand bond strengths are excellent candidates to achieve alcohol dehydrogenation reactions, as net oxidation requires dihydrogen loss from the metal. Pincer ligands have been shown to promote excellent stability and reactivity in acceptorless alcohol dehydrogenation reactions with first-row transition metal complexes, and metal-ligand cooperativity that has been successful using PGM catalysts, which may also be investigated for the base metals as the project progresses.

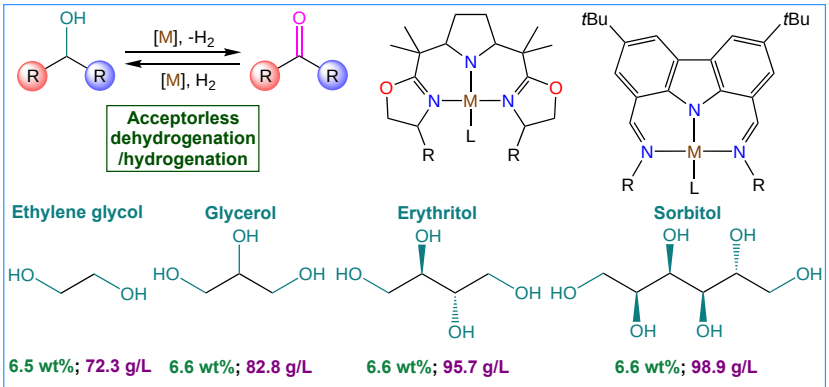

Figure 1. Example reaction, complexes and alcohol substrates, with their theoretical gravimetric and volumetric hydrogen capacities with acceptorless alcohol dehydrogenation.

Our recent research has revealed that complexes featuring cheap, non-toxic and earth abundant base metals can catalyse a range of reactions, including dehydrogenation and hydroelementation reactions. In terms of the proposed alcohol substrates, we envisage challenges such as differing reactivity with substitution at the hydroxyl residues and the catalysis of the reaction with H_2 (reverse reaction), allowing a closed cycle for LOHC technology. Judicious choice of catalyst (or pre-catalyst), including

the metal and ligand, and reaction conditions will facilitate the acceptorless alcohol dehydrogenation reactions with efficiency and product selectivity. Determination of reaction mechanisms through spectroscopic, structural and kinetic investigations allows the optimisation of the reactions. It is envisaged that investigations will also allow improvements in the temperatures, solvents (including a range of biomass-derived solvents) and catalyst loadings required for hydrogen release, but also the selectivity (*e.g.* avoidance of any undesirable by-products). The student will benefit from training in chemical techniques (*e.g.* organometallic chemistry, spectroscopy, crystallography and kinetic investigations) and principles of sustainable chemistry.

Deliverables

- New earth abundant catalysts for acceptorless alcohol dehydrogenation/hydrogenation reactions
- Mechanistic understanding for these reactions, allowing improvements in LOHC technologies
- Optimisation of routes to hydrogen release from biomass-derived materials

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Supported nanoalloys for sustainable hydrogen production

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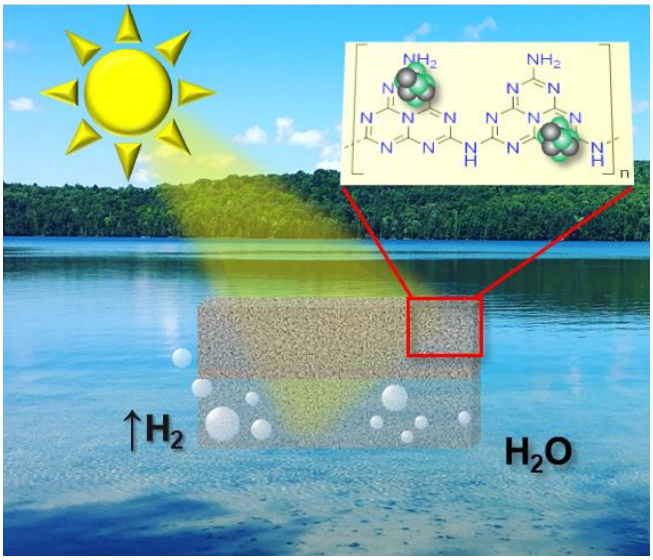
Project description

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.

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

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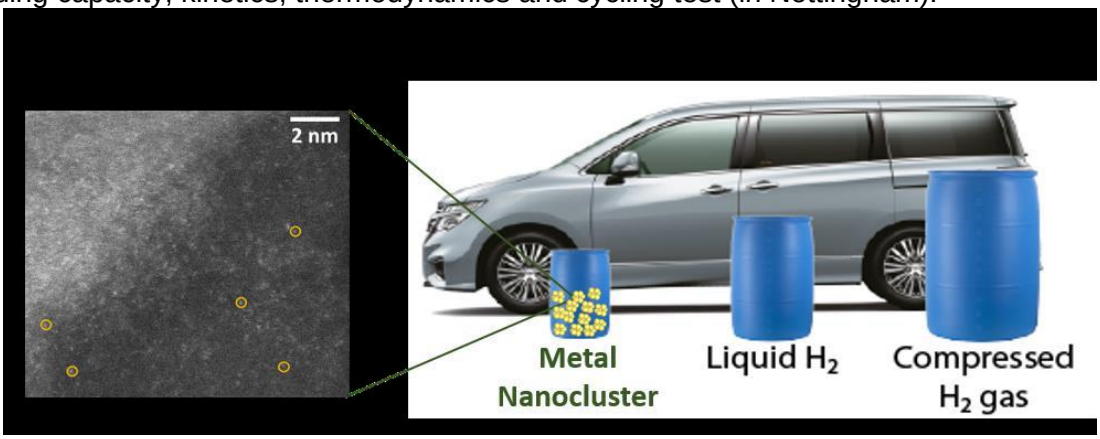
Project description

The development of volumetric efficient solid-state hydrogen (H2) storage materials is crucial for decarbonisation in the transport sector. As one of the most promising H2 storage materials, the advantages of magnesium hydride nanoparticles includes their high H2 storage capacity (7.6 wt.%) and low cost ($3/kg). However, slow kinetics and a high working temperature (ca. 250 ºC) limit its commercial application for on-board H2 storage. In order to improve its properties (higher kinetics, lower temperature), this project will utilise metal nanoclusters (MNCs), which are fundamentally different compared to more widely used metal nanoparticles (diameters >2 nm), where the majority of metal atoms remain 'hidden' within the lattice and are excluded from participation in useful chemistry. In contrast, the majority of the atoms in MNCs are fully accessible for physicochemical processes, while new functional properties, inaccessible in bulk metals or in nanoparticles, can emerge as a result of confinement in MNCs. Theoretical calculations predict that nano-tuning could reduce the (de)hydrogenation reaction energy when NCs of Mg/MgH2 are used, therefore reducing the working temperature [JACS, 2005, 127, 16675-80]. This would substantially reduce the on-board H2 storage cost enabling their use in fuel cell vehicles for zero-emission transport. This is a collaboration project between University of Nottingham and Diamond Light Source.

The specific steps will involve: (i) synthesis of graphitic carbon nitride (*g*-C3N4), which is an ideal support for stabilisation of MNCs due to its nitrogen "cavity" (Nottingham), (ii) depositing a series of MNCs with different sizes and composition (i.e. Mg and Pd, and their nano-alloys) on *g*-C3N4 and their characterisation: AC-STEM including chemical mapping and depth profile, and XPS / NAP-XPS in Diamond, (iii) Investigating the electronic changes on MNCs under H2 environment at different temperatures (AC-STEM and NAP-XPS in Diamond), (iv) evaluation of H2 storage properties including capacity, kinetics, thermodynamics and cycling test (in Nottingham).



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Stakeholder collaboration: Diamond

Deliverables

- Fabrication of MNCs with atomically precise size and composition (focus on Mg, Pd and their nano-alloys).
- Analytical approaches delivering atomic-level dynamic information for MNCs in ex-situ, in-situ and operando conditions (H2 atm with different temperatures up to 350 ºC with focus on NAP-XPS and STEM).
- Design a protocol for metal clusters investigations under hydrogen for I09-XPS/NAP-XPS and STEM.
- Provide new links between Sustainable Hydrogen CDT, I09, ePSIC, Ammonia Demonstrator and Nottingham.

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

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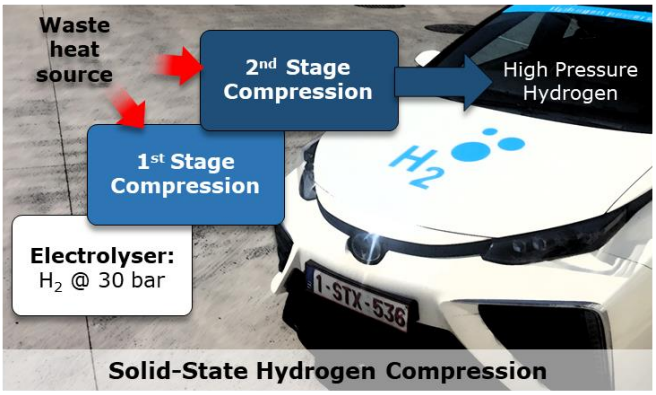
Project description

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 ^{o}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.



Solid-State Hydrogen Compression

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.

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Nanostructured hydrogen storage materials for offshore green hydrogen

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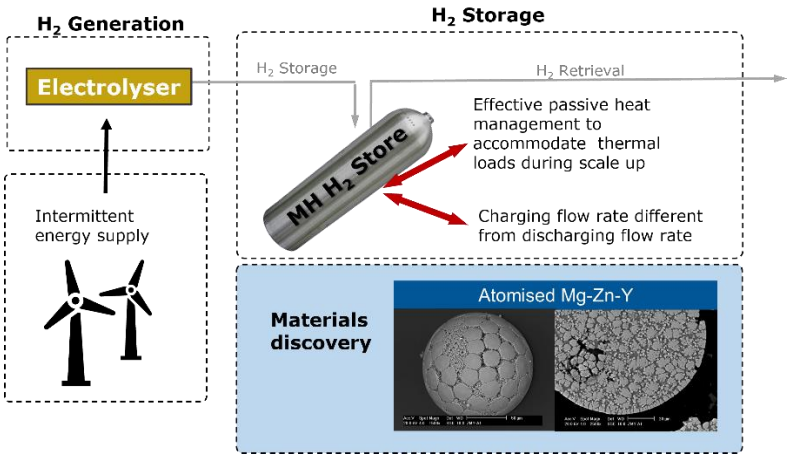
Project description

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.

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

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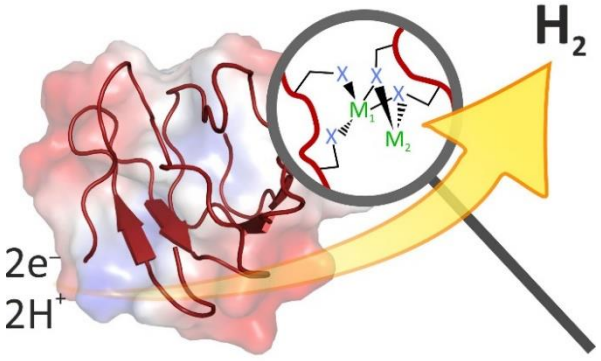
Project description

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

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Efficient Hydrogen Separation using Proton-Conducting Ceramic Membranes and Electrochemical Cells

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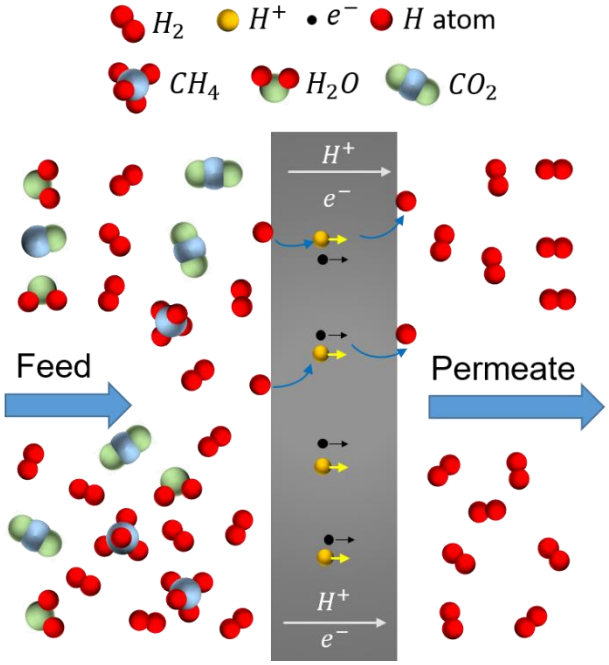
Project description

To achieve energy-efficient and low-cost hydrogen separation using proton conducting ceramic membranes for hydrogen rich streams generated through reforming of natural gas as well as onsite purification of hydrogen close to the point of end use for dilute hydrogen streams distributed through natural gas pipelines using ceramic proton electrochemical cells (hydrogen pumps). Hydrogen plays a vital role in helping the UK meet its 2050 target of net-zero greenhouse gas emissions through decarbonisation of its energy system including electricity, transport and heating sectors. Most hydrogen used today is produced from fossil fuels (e.g., through steam reforming of natural gas, coal gasification). The product gases consist mainly of H_2 and CO_2, as well as other impurity gases such as CH_4, and CO. Therefore energy-efficient and low-cost hydrogen separation constitutes a crucial process to more toward to hydrogen economy.

Dense ceramic membranes made of mixed protonic-electronic conductors (MPECs) are capable of separating hydrogen from the gas mixtures with 100% selectivity, reduced energy penalty and cost compared to the well-established techniques such as the pressure swing adsorption technique. Ceramic proton conductors can also be used to fabricate electrochemical cells (hydrogen pumps) to obtain high purity hydrogen from dilute hydrogen streams when the existing hydrogen separation techniques become highly inefficient and costly. This is particularly important to facilitate distribution of hydrogen using existing natural gas pipelines. The ceramic proton electrochemical cells could enable extraction of high purity hydrogen from the natural gas blend with 10-20 vol% hydrogen close to the point of end use.



Deliverables

- New proton conductors with high proton conductivity and stability under operation conditions.
- New high performance and stable mixed protonic-electronic conductor ceramic membranes with H_2 permeability > 1.0 mL cm^{-2} min^{-1} at 700− 1000 °C with a 1 bar pressure gradient meeting commercial requirements.
- Ceramic proton electrochemical cells exhibiting high H_2 separation rate > 5.0 mL cm^{-2} min^{-1} under 1.0 V at 300−500 °C with the Faraday's efficiency above 98%.

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Highly efficient molecular hydroge-evolution catalysts

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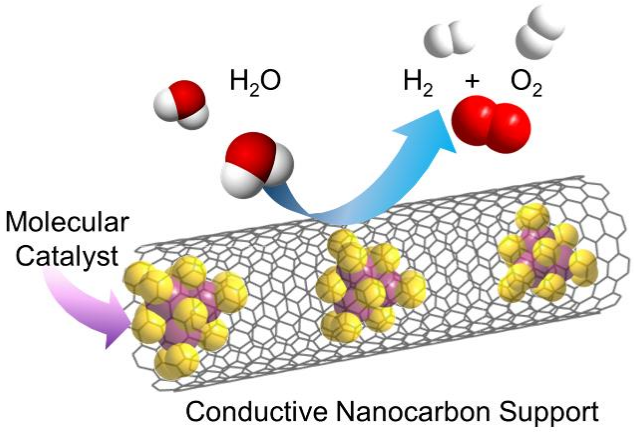
Project description

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.



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.

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Water splitting beyond the volcano plot

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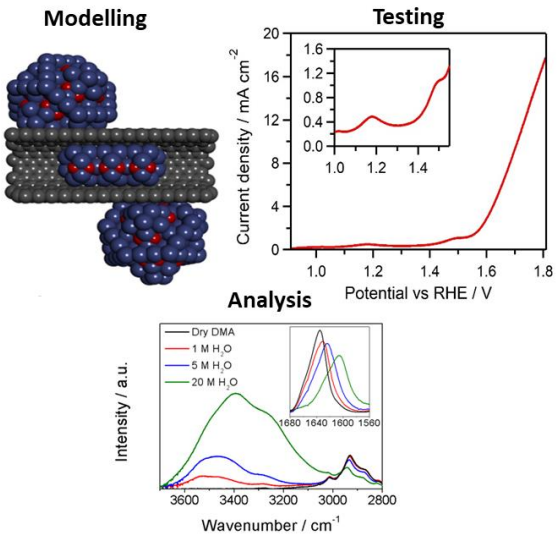
Project description

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.

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H2COOL - dual energy store for refrigerated transportation

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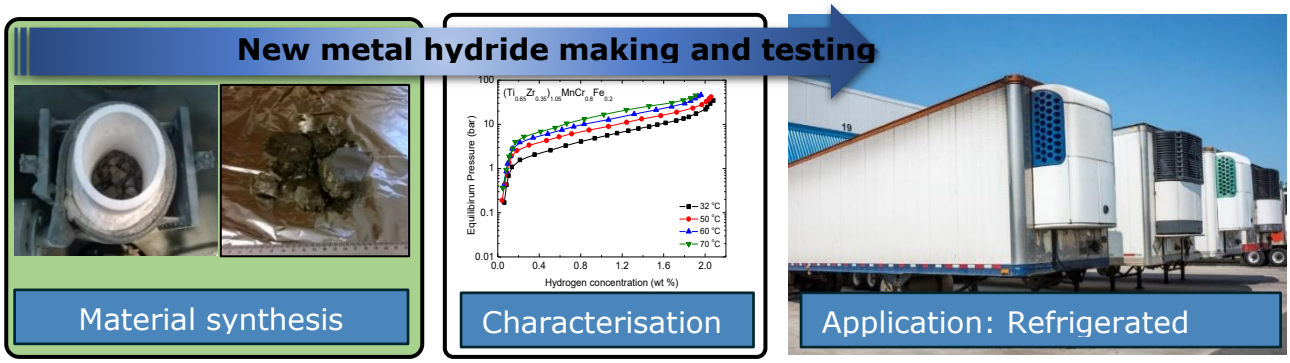
Project description

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.



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.

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Sustainable catalysts for low temperature and pressure ammonia synthesis

Gavin Walker, Marcus Adams and Matthew Wadge
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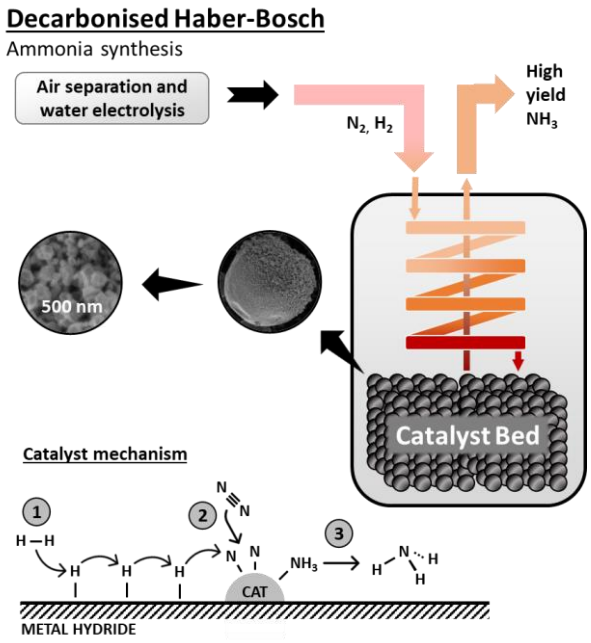
Project description

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.

Sustainable Hydrogen
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Decarbonised Clean Heavy Duty Engines via Hydrogen and Ammonia Flex Fuelling

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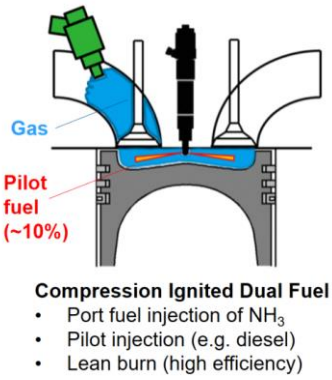
Project description

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



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

Sustainable Hydrogen
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Machine Learning Discovery of Electrocatalysts for Sustainable Hydrogen Production

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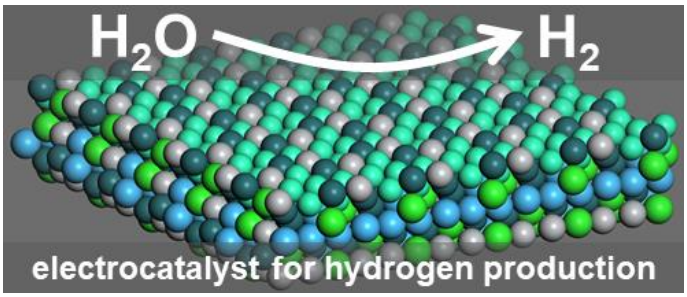
Project description

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.



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

Sustainable Hydrogen
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Green hydrogen production from water splitting powered by renewable electricity

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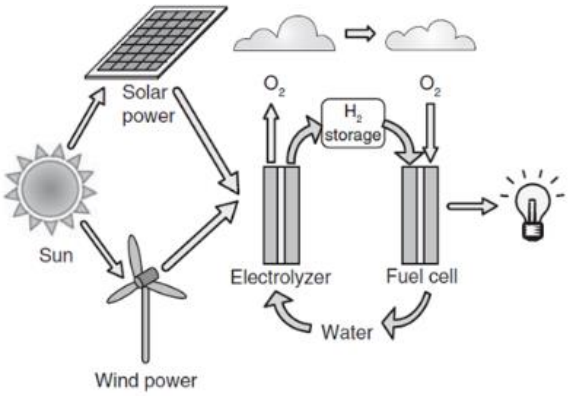
Project description

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

LONGHU 龙湖科技 Longhu Sci. & Tech.

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Metal membranes for separating pure hydrogen from gas grids

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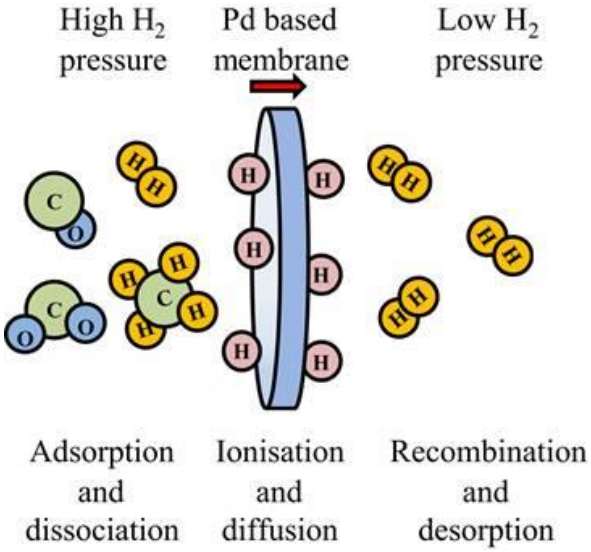
Project description

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)

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Proton exchange membrane water electrolysers with thin film nanostructured electrodes

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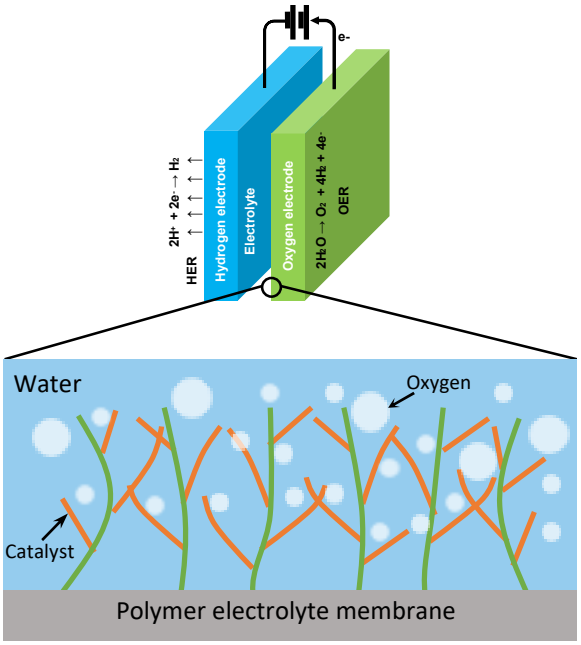
Project description

The biggest challenge with current proton exchange membrane water electrolysers (PEMWE) is their poor power performance and durability, which is mainly caused by large mass transfer losses and degradation of the electrode structure from the random electrode structure from catalyst nanoparticles. In this PhD project, we'll develop a new generation of catalyst electrodes from aligned IrO_2- and metal oxide-based nanowires for PEMWE applications, taking the advantages of the high stability of nanowires and the boosted mass transfer characteristics of the unique thin catalyst layers from nanowire arrays.



Deliverables

- Substrate surface modification approach to increase the surface activity.
- In-situ nanowire array growing process based on IrO_2 and metal oxide materials.
- Surface deposition technique of $SrIrO_3$ on nanowire arrays.
- Electrode evaluation using both half-cell and single cell test.

Sustainable Hydrogen
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Modified transition metal catalysts for hydrogen and oxygen evolution

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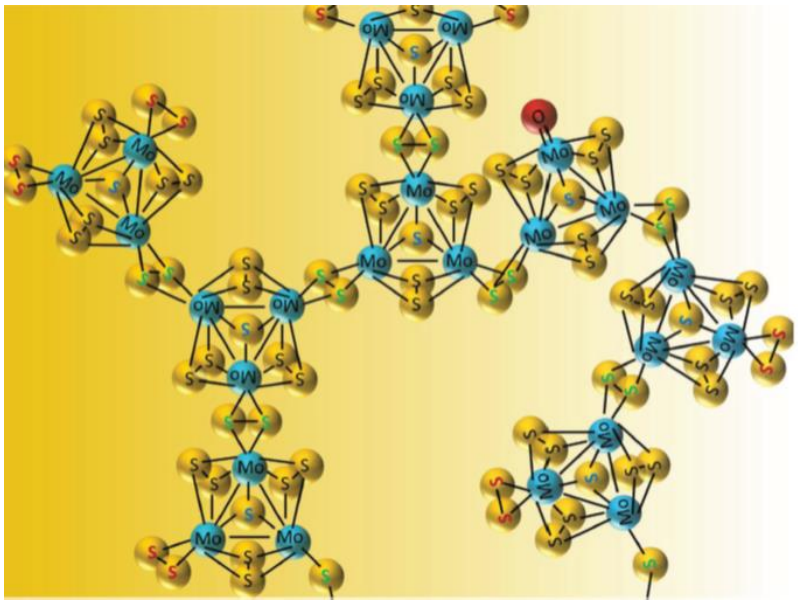
Project description

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
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Business cases for Green Hydrogen

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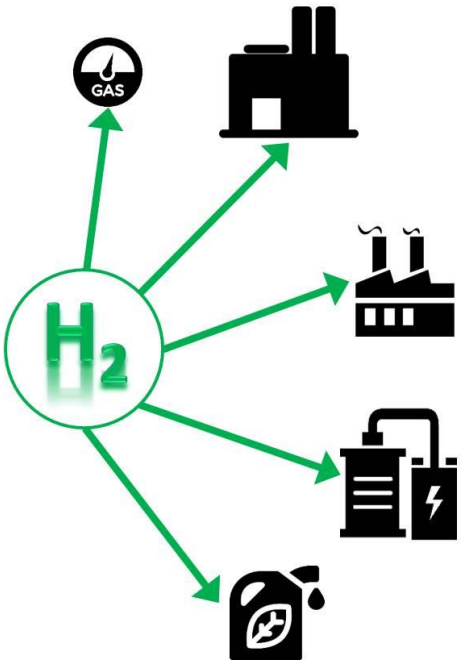
Project description

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

Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

Safety of liquid and cryogenic hydrogen in energy applications

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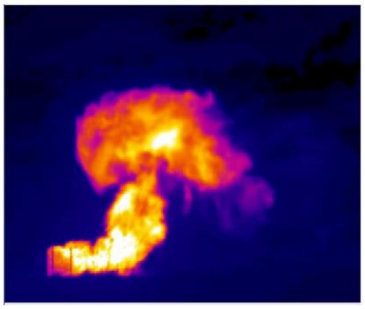
Project description

Liquid hydrogen (LH2) is the most efficient way to transport hydrogen to destination at the initial stage of deployment of hydrogen systems and infrastructure when dedicated pipelines are not yet available. The development of innovative safety strategies and engineering solutions for LH2 systems and storage infrastructure requires understanding of underlying physical phenomena, development and validation of contemporary (CFD) and reduced engineering models and tools for safety design. The models and engineering solutions to prevent and mitigate incidents involving LH2 systems and infrastructure have to be developed further. Research areas include but not limited to the following phenomena: cryogenic and multiphase release and dispersion from LH2 storage system in the open atmosphere and confined spaces; mitigation of pressure and thermal hazards from releases of cryo-compressed hydrogen (CCH2); conditions for explosion in LH2 spills; rupture, pressure and thermal effects after LH2 tank rupture in a fire including BLEVE; etc. The suitability of available hydrogen safety engineering tools for assessment of LH2 storage safety, including in conditions of flight, should be critically analysed. New analytical tools and numerical models for assessment of consequences for LH2 and cryogenic hydrogen storage should be developed based on an improved understanding of the underlying physics. The developed models must be validated against experimental data that was obtained within EU pre-normative research project PRESLHY and other national projects.

Dispersion of LH_2 release



LH2 release fireball

Deliverables

- Theoretical and/or numerical models for assessment of hazards associated with LH2 systems and infrastructure
- Validation of theoretical and/or numerical models against experimental data

Sustainable Hydrogen
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Safety strategies and engineering solutions for hydrogen heavy-duty vehicles

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Project description

Strategic political developments towards a low carbon economy enable practical implementation of zero-emission applications including hydrogen-fuelled heavy-duty vehicles (HDV) such as buses and trucks. The use of hydrogen in public transport implies stringent requirements of bus design. Not all knowledge gaps are closed to manufacture inherently safer HDV transport, including double-deck buses. Industry and regulators have particular concerns about two aspects of HDV design that are considered critical for their successful roll-out:
- development of refuelling protocol for heavy-duty vehicles capable to provide refuelling time comparable with modern fossil-fuel vehicles and yet not jeopardising the safety of onboard compressed hydrogen storage system (CHSS), and
- fire-resistance rating of current CHSS, which may lead to their rupture in a fire with catastrophic consequences, i.e. blast wave, fireball and projectiles.

The project will critically review “old” and new hazards of HDV of different designs and sectors, i.e. buses and trucks. Existing prevention and mitigation safety strategies and engineering solutions, knowledge gaps and technological bottlenecks in the provision of safety of HDV will be identified and analysed. The expected research outcomes may be in the form of:
- recommendations for the inherently safer design of HDV;
- fuelling protocol for different CHSS;
- optimised safety design of CHSS using TPRD;
- safety design of CHSS based on self-venting TPRD-less containers.

It is envisaged that the research will rely on the use of Computational Fluid Dynamics (CFD) to study and optimise the heat and mass transfer during refuelling, the performance of CHSS in realistic fires of different intensity, including smouldering and impinging jet fires. The successful candidate is expected to have a strong background in one of the following disciplines: mathematics, physics, chemistry, fluid dynamics, heat and mass transfer, combustion. Any previous experience of 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-

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processor workstations available at HySAFER Centre and HPC facility available within EPSRC KELVIN-2 project. This research will be aligned to HySAFER's externally funded projects and reported at international conferences. Publication of results in peer-reviewed journals is expected.

Deliverables

- Development and validation of models for assessment of hazards
- Simulations of selected scenarios and development of mitigation strategies
- Development of fuelling protocols selected CHSS of HDV

Sustainable Hydrogen
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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

Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

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.

www.dnv.com/expert-story/maritime-impact

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 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.