

Modelling Hydrogen Storage in Quasi-Crystals

Elena Besley, Xuanli Luo and Gavin Walker

University of Nottingham

Email: Elena.Besley@nottingham.ac.uk

Project description

The aim of this project is to investigate computationally the main physical properties that nanometre size quasi-crystals (QCs) inherit from the absence of periodicity and to investigate their potential in a few foreseen applications, notably in hydrogen storage and sustainable hydrogen production.

Amongst complex metallic alloys the atomic structure of a QC is without a doubt the most difficult to solve, however a number of stable QCs are now known (see an example of the ternary icosahedral Zn-Mg-Tm QC in figure 1). Of these new QCs, none were comprehensively studied from the standpoint of their potential applications, with the exception of some studies on the Ti-Zr-Ni system that shows potential for hydrogen storage (figure 2).

This project will assess computationally a wide range of QCs for their suitability as a novel hydrogen storage material and as a novel QC catalyst replacing current expensive Pt based catalysts in electrocatalytic water splitting. The project will re-launch the quest for inexpensive materials for energy applications with superior performance by utilising the computational methods, recently developed in the E. Besley's group, for understanding gas interactions, separation and diffusion in solid materials.

This computational modelling will guide the synthesis of new QC formulations and their testing in hydrogen storage and electrocatalytic applications.

Deliverables

- Computational prediction of nanometer size quasi-crystal (QC) thin films and clusters with precisely controlled size and structure;
- Computational modelling of hydrogen uptake of the QCs
- Comparative computational study of the catalytic properties of QCs and Pt-based catalysts with a focus on water splitting.

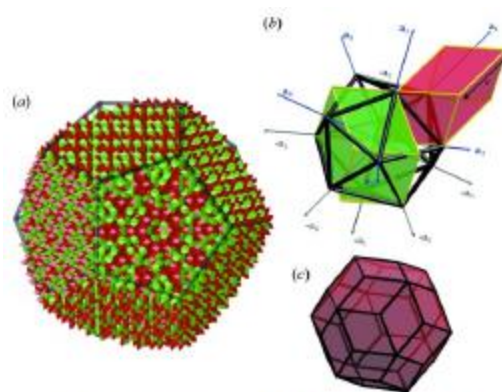


Figure 1: Atomic structure of the ternary icosahedral Zn-Mg-Tm quasicrystal (*Acta Cryst* 2020)

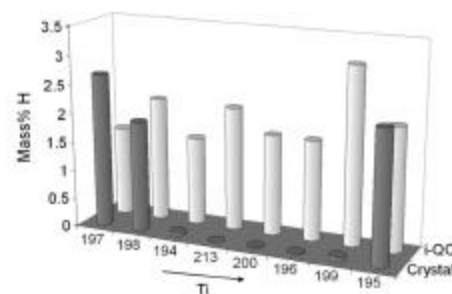


Figure 2: Mass change upon hydrogen loading of crystalline (front) and icosahedral quasicrystal (back) Ti-Zr-Ni alloys at constant Ni content and variable Ti/Zr ratio (*ChemSoc.Rev* 2012)

Nano-Quasicrystals for Hydrogen Storage

Xuanli Luo, Elena Besley and Gavin Walker

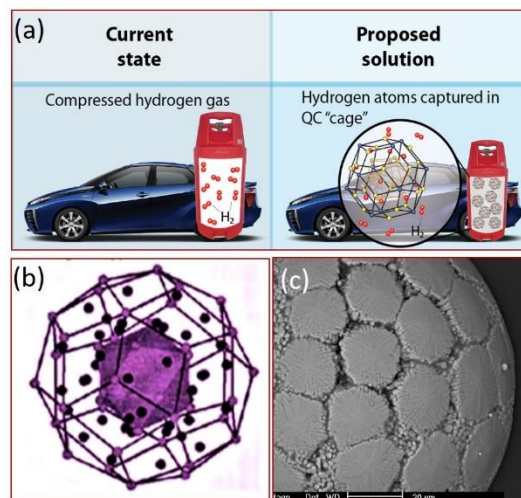
University of Nottingham

Email: Xuanli.Luo@nottingham.ac.uk

Project description

Producing only water as a waste product, sustainable hydrogen could offer credible decarbonisation solutions for energy supply, transport, commercial and domestic sectors. A major barrier to exploitation of hydrogen in energy applications especially vehicles is the lack of a safe, efficient and cost-effective storage system. Quasicrystal (QC) have potential to be a lightweight hydrogen storage material due to their unique multi-shell cluster structure, which provide a high density of interstitial sites to accommodate hydrogen. For example, the typical storage capacity is less than 2H/M (hydrogen atom per metal) in conventional metal/alloy hydrides, in comparison to 3.2 H/M of the theoretical capacity in QC hydrides. A wide range of advanced crystal materials have been investigated for hydrogen storage; yet little is known about QC with respect to energy storage, especially nano-sized QCs

This project aims to develop high-performance nano QC materials for on-board vehicle hydrogen storage. The student will synthesize nano QC via various synthetic methods, such as chemical vapour deposition and physical vapour deposition. The characterisation via XRD, SEM, TEM will reveal the structure of nano QCs. Hydrogen storage properties including capacity, kinetics, thermodynamics and reversibility will be evaluated by differential scanning calorimetry, thermogravimetric analysis, and pressure-composition-isotherm techniques. Working alongside a computational project led by Prof E. Besley, this project will also study the interaction between hydrogen atom and host QC lattice via in-situ powder neutron diffraction to understand the relationship between structure and storage performance, therefore set the design protocol for nano QCs for hydrogen storage.



(a) It is proposed to use quasicrystals for on-board hydrogen storage, which is safer with higher volumetric efficiency compared to compressed gas. (b) Quasicrystal have potential to be a lightweight hydrogen storage material due to their unique multi-shell cluster structure which contains enormous hydrogen-favoured interstitial sites (represented by dark dots). (c) SEM image of Mg-based quasicrystals.

Deliverables

- Synthesize nano-sized quasicrystals suitable for hydrogen storage with focus on Mg-based, Ti-based QC and Test the hydrogen storage properties
- Conduct in-situ experiments including neutron diffraction to investigate the interaction between hydrogen atom and host QC lattice
- Set the design protocol for using nano QCs for hydrogen storage

Advanced Hydrogen Sensing Platform Based on Functionalized Metal-Organic Frameworks

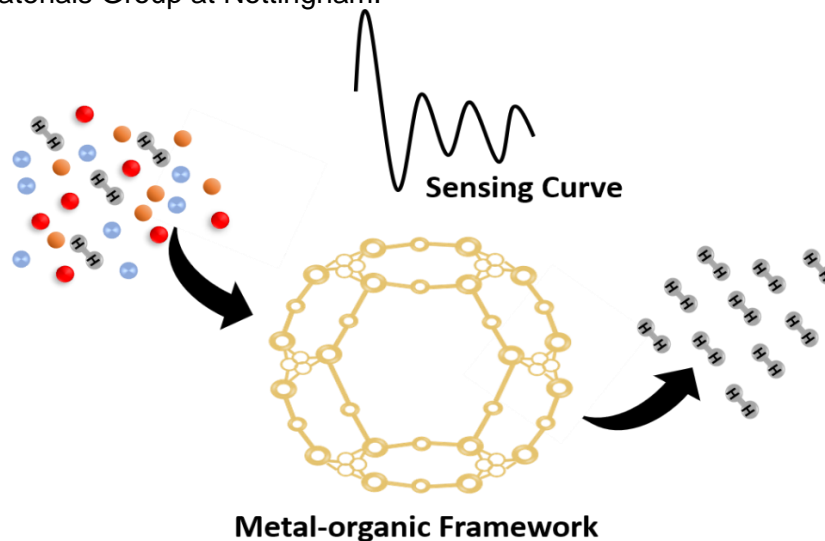
Oluwafunmilola Ola, Gavin Walker and Elena Besley

University of Nottingham

Email: Oluwafunmilola.Ola1@nottingham.ac.uk

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.

Base Metal Catalysis of Acceptorless Alcohol Dehydrogenation for Hydrogen Storage

Deborah Kays and Pete Licence

University of Nottingham

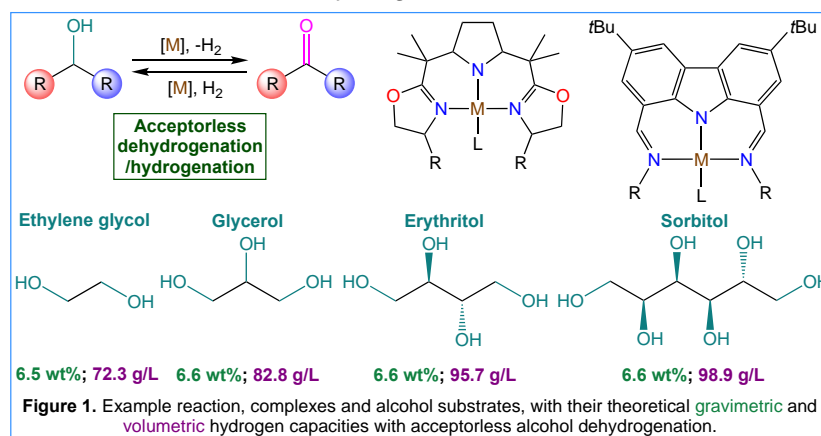
Email: Deborah.Kays@nottingham.ac.uk

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 C₄–C₆ 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 H₂. 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.



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 H₂ (reverse reaction), allowing a closed cycle for LOHC technology. Judicious choice of catalyst (or pre-catalyst), including



Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

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



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

Jesum Alves Fernandes, Xuanli Luo, David Grant, Thomas Slater and David Duncan

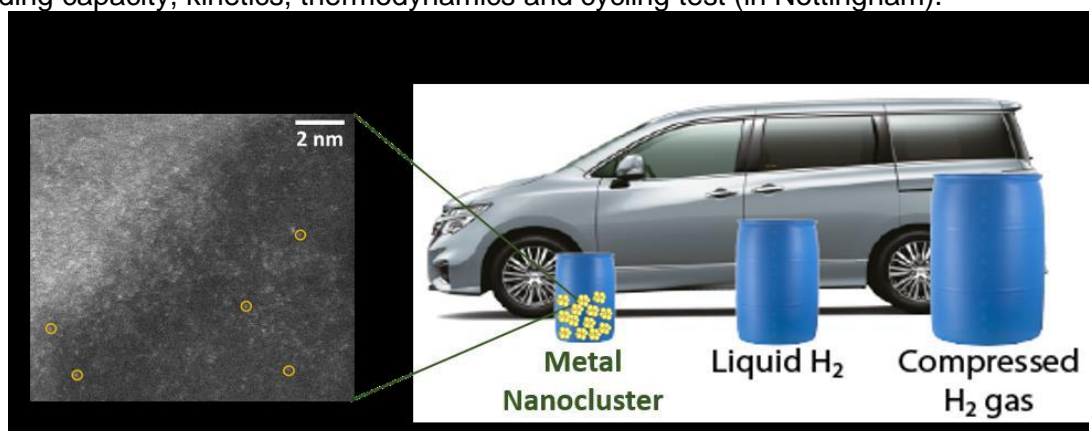
University of Nottingham

Email: Jesum.Alvesfernandes@nottingham.ac.uk

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 °C) 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).





Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

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 °C 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.

Modular Additive Manufacturing for Next-generation Hydrogen Storage

Ian Maskery and Gavin Walker

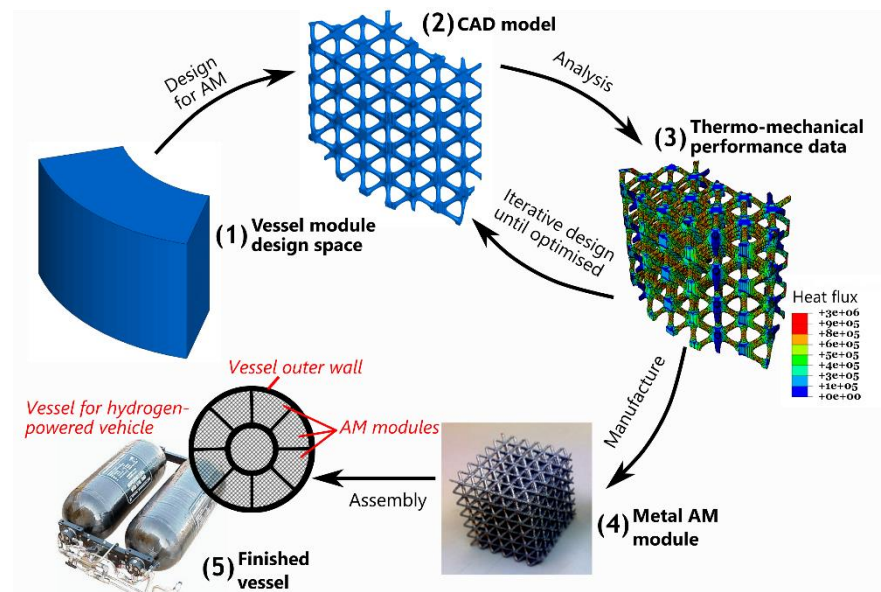
University of Nottingham

Email: Ian.Maskery@nottingham.ac.uk

Project description

Compact hydrogen storage is a major challenge for hydrogen powered vehicles, with current state-of-the-art storage vessels being too large and operating at dangerously high pressures. Solid state metal hydrides (MH) can store large quantities of hydrogen in much smaller volumes and at lower pressure. However, MH stores have not made it to market because suitable vessels have not yet been developed. This project will investigate the design and manufacture of a new type of compact MH storage vessel – the *Type S* vessel. It will perform multiple functions, including heat management (due to exothermic and endothermic charging and discharging cycles), and MH bed breathing (due to MH expansion and contraction whilst cycling). To address these requirements, the project will use metal additive manufacturing (AM) in an entirely new way, using individual latticed sub-components, or modules, which are joined together to create the vessel interior. By the end of the project, the student will have successfully demonstrated this new design and manufacturing approach for MH storage applications.

The student will investigate this modular manufacturing approach with a combination of AM processing and metrology, numerical modelling (e.g., finite element analysis), and component-level testing (e.g., microstructure analysis, joint strength and leak testing). They will gain a broad set of skills and knowledge relevant to modern design and analysis techniques, as well as manufacturing and materials science.



Deliverables

- Through the investigation of the modular lattice design approach, the project will generate structure-performance relationships which will underpin a novel computational AM design toolkit. This will be configurable for a range of thermo-mechanical applications throughout the renewable energy, automotive and aerospace sectors.
- Reduced scale *Type S* vessel prototypes will prove the manufacturing concept, the effectiveness of the *in situ* joining methods, detect outstanding technical challenges and provide cost and performance data for the project partner and future stakeholders.

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

Ming Li, Begum Tokay and David Grant

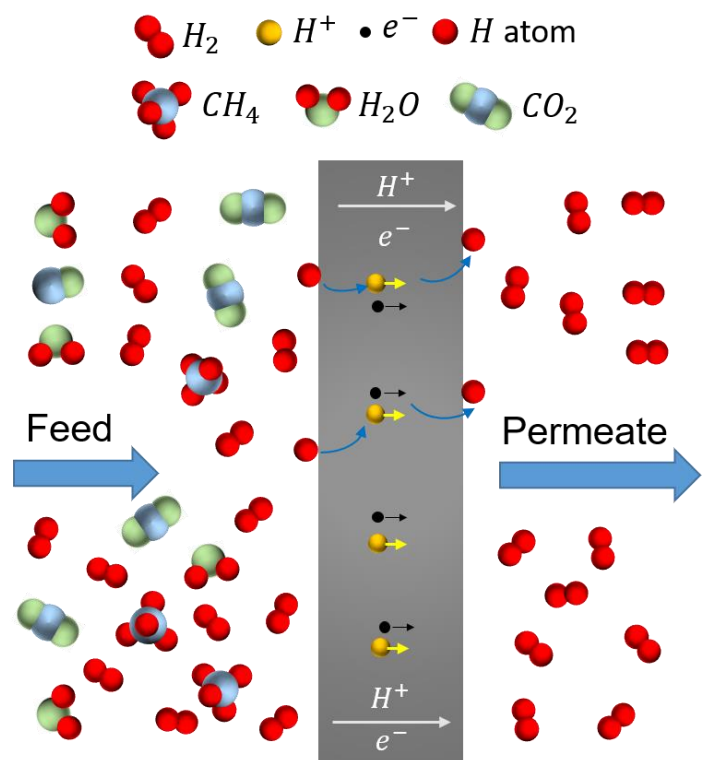
University of Nottingham

Email: Ming.Li@nottingham.ac.uk

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 move toward a 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 $> 1.0 \text{ mL cm}^{-2} \text{ min}^{-1}$ at 700– 1000 °C with a 1 bar pressure gradient meeting commercial requirements.



Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

- Ceramic proton electrochemical cells exhibiting high H₂ separation rate > 5.0 mL cm⁻² min⁻¹ under 1.0 V at 300–500 °C with the Faraday's efficiency above 98%.

Innovative compression technologies for hydrogen storage and distribution

David Grant, Alastair Stuart, Kandavel Manickam and Gavin Walker
 University of Nottingham
 Email: David.Grant@nottingham.ac.uk

Project description

Both the UK Government, and the European Union recognise hydrogen as a potential solution for decarbonising hard to reach sectors, including heat, transport and industry. Hydrogen is part of UK's ten point plan for green industrial revolution. The successful establishment of a hydrogen-based energy infrastructure will be reliant upon the development of efficient H₂ storage and distribution technologies. Conventionally, hydrogen is stored at high pressures typically 20 MPa (200 bar) or greater but to compress hydrogen mechanically requires an additional (ca. 20%) input of energy. The solid state compression of hydrogen offers a more economical alternative to mechanical compression with a higher level of safety and significantly lower maintenance regime.

At UoN, a prototype solid state compressor has been built as part of an EPSRC funded project. The prototype was initially developed to demonstrate the concept of refuelling H₂ Fuel Vehicles in a domestic setting but there is now growing interest from other sectors. It is proposed to develop the scope of solid state compressor technologies through consultation with relevant industries. Once a target application has been identified the challenge will be to optimise the existing prototype to provide operational data and demonstrate the potential of the technology.

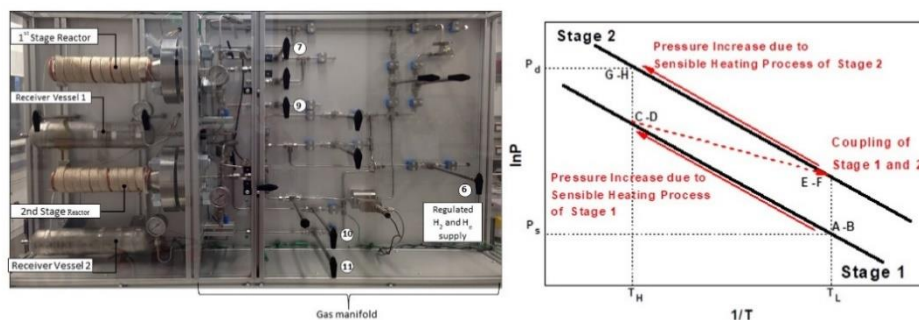


Fig. 1 Photograph of the prototype system and working principle schematic of the two stage hydrogen solid state compressor

Deliverables

- Performance evaluation of existing solid state compressor prototype.
- Identification of potential commercial applications through industrial engagement.
- Design modifications to prototype system to enable it to meet and new requirements of the target operating scenario requirements.
- A portfolio of operational data to evidence commercial potential of technology for target application.



Highly efficient molecular hydroge-evolution catalysts

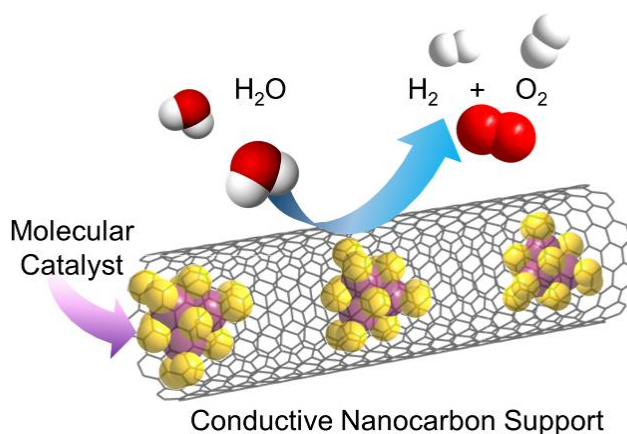
Graham Newton and Lee Johnson

University of Nottingham

Email: Graham.Newton@nottingham.ac.uk

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.



Water splitting beyond the volcano plot

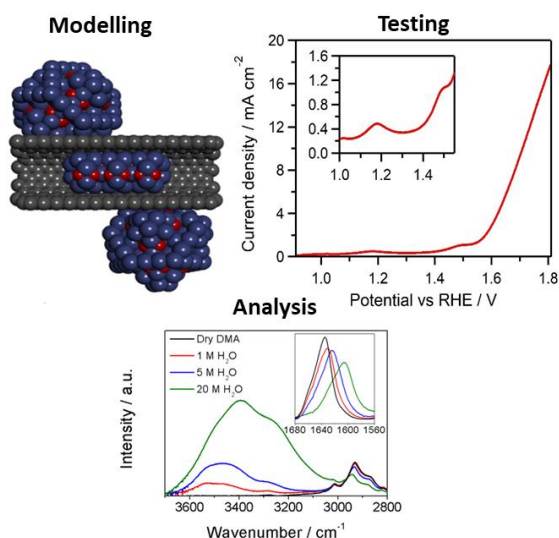
Lee Johnson, Darren Walsh and Graham Newton

University of Nottingham

Email: Lee.Johnson@nottingham.ac.uk

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 H₂O electrolysis compared to conventional aqueous based systems.
- First prototype demonstration.

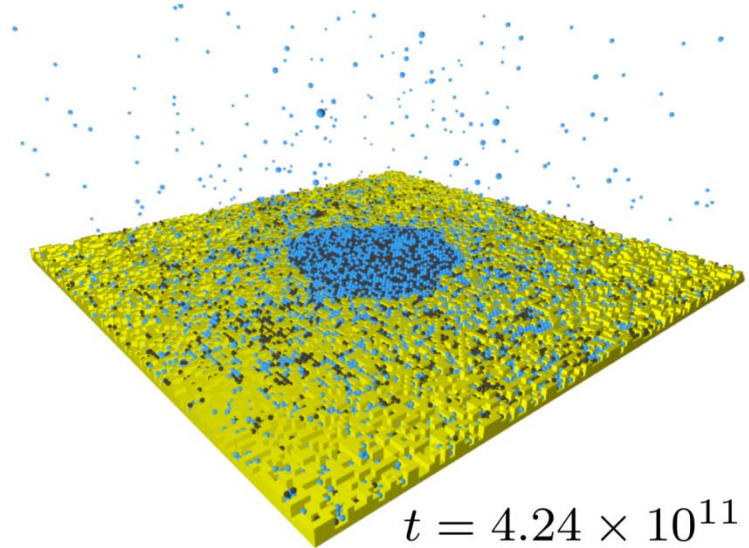


Modelling hydrogen storage in porous solids

Pooja Goddard and Andy Archer
Loughborough University
Email: P.Goddard@lboro.ac.uk

Project description

Hydrogen has great potential as a fuel, however this relies on it being stored in a way that it has a high enough volumetric energy density. To put it simply, to compete with gasoline, there must be enough fuel in the tank to travel ~500miles and the tank should be comparable in size and weight with conventional gasoline storage tanks. To get to the volumetric energy densities required, storage in various porous materials, such as carbon nanotubes, activate carbon, MOFs, Mesoporous Silica, Zeolites and others, have been suggested. In this project we will develop a model for the adsorption and transport of hydrogen within such structures. The initial focus will be on the interplay between the shape/geometry of the structures and how that influences maximum hydrogen adsorptions and rates at which the hydrogen can enter/leave the structure. The model will be based on dynamical density functional theory and/or kinetic Monte-Carlo modelling. To bridge the length-scales we will develop some coarse-grain lattice models, where such models were developed for modelling the transport and drying of inks on rough surfaces. The project will allow materials researchers to focus on those structures which are most efficient and should lead to identifying particular porous material architectures that are best for hydrogen storage.



Deliverables

- A multiscale (computational) model for hydrogen adsorption and transport in porous materials
- Improved understanding of the behaviour of hydrogen in a variety of porous materials
- Optimal control of structure/property relationships e.g. relation between material geometry and transport properties



Evaluation of sustainable hydrogen production from wastewater with renewable energies

Eileen Yu, Upul Wijayantha and Jin Xuan

Loughborough University

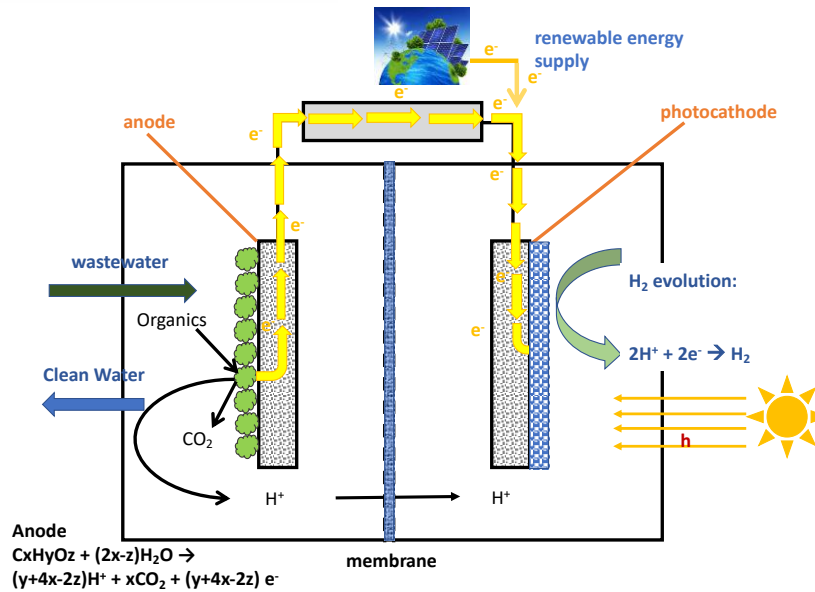
Email: E.Yu@lboro.ac.uk

Project description

UK has a legal obligation to achieve net-zero greenhouse gas emissions by 2050. Hydrogen will be an important component in our quest for transition to low-carbon or zero-carbon energy network. Currently hydrogen is mostly produced through petrochemical route with Steam Methane Reforming, which has high carbon footprint and not sustainable. Other technologies, such as Catalytic Methane Decomposition from biomass, electrolysis and Solar water splitting have demonstrated potentials utilising renewable resources. However, the cost for expensive catalysts and materials, as well as high energy demands are challenges to tackle. Currently Water industry is consuming 3% of UK's electricity for aerating, pumping and treatment of wastewater, the fourth most energy-intensive sector in the UK. It is responsible for 5% of the 200 million tonnes/year of greenhouse gas emission in the UK. On the other hand, the internal chemical energy of mixed wastewater is around 16.8 MJ/tonne, and domestic wastewater has 7.6 MJ/tonne. With 11 million tonnes of wastewater collected everyday in the UK, the energy in the total wastewater could be up to 51.3 GWh/day.

Bioelectrochemical systems (BES) are emerging technology use whole microorganisms as the biocatalysts to harness energy in wastewater by oxidising organic matter to generate electrons which flow between the anode and cathode. The electrons and protons produced are used on the cathode for reduction reactions, such as hydrogen evolution (HER) in microbial electrolysis cells (MECs), resulting in reduced overall energy demand for hydrogen production. From our previous research, while removing organic matters from wastewater, the bioanode is able to provide 1/3 of energy required, or reduce overpotential up to 200 mV for hydrogen production. However, the current density of MECs is low and resulted in low hydrogen yield. The rapid development of photoelectrochemical systems (PEC) utilising solar energy provides a possible solution with hybrid system combining MEC and PECs harnessing the synergy from both waste and solar energy. Recent study showed 23mA/cm² was achieved with such hybrid system without additional electricity input, which makes this a promising technology with potential for large scale applications.

In this project, technology development on novel materials and reactor designs to achieve high efficiency and yield in HER with wastewater and low cost materials will be investigated; evaluation of this technology in terms of life cycle assessment (LCA) and technology economic assessment (TEA) to compare the technology with other hydrogen production technologies will also be conducted using the data from technological study. Our industrial partners Chivas Brothers and Shell Research will be actively involved in the project development and progress by providing wastewater samples, access to the manufacturing sites, providing data and access to Shell Biological lab. We envisage the project not only advancing technology for water industry with low cost, sustainable system simultaneously treating wastewater and efficiently generating hydrogen, but also providing reasoning and understanding of the influence of the novel technology, in terms of carbon budget and social economic impacts to change high energy demand and carbon emission industrial sectors towards Net zero and achieving clean growth.



Deliverables

- Providing multidisciplinary training to a PhD student with skills in Engineering, chemistry, biotechnology and social economics, problem solving and critical analysis at the SuSHy CDT.
- Design and prepare reactors for hydrogen production with BES and PEC.
- The work will provide feasibility and evidence for further collaborative with water industry and larger UKRI proposals.

Metal membranes for separating pure hydrogen from gas grids

David Book, Shahrouz Nayeboossadri and Rex Harris

University of Birmingham

Email: d.book@bham.ac.uk

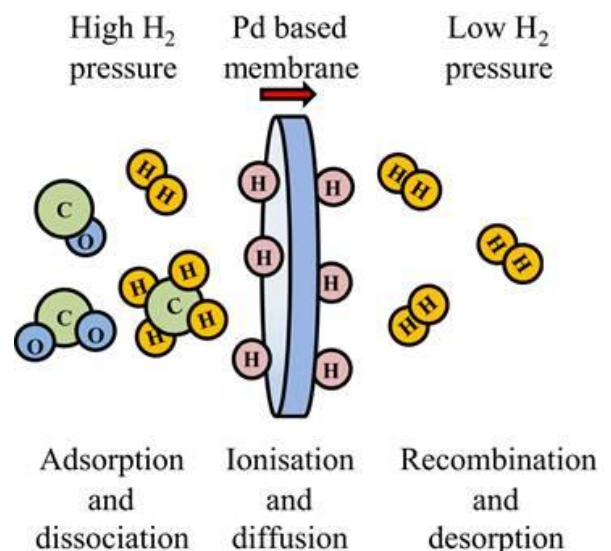
Project description

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 (CH₄/H₂ and H₂ grids)

Proton exchange membrane water electrolyzers with thin film nanostructured electrodes

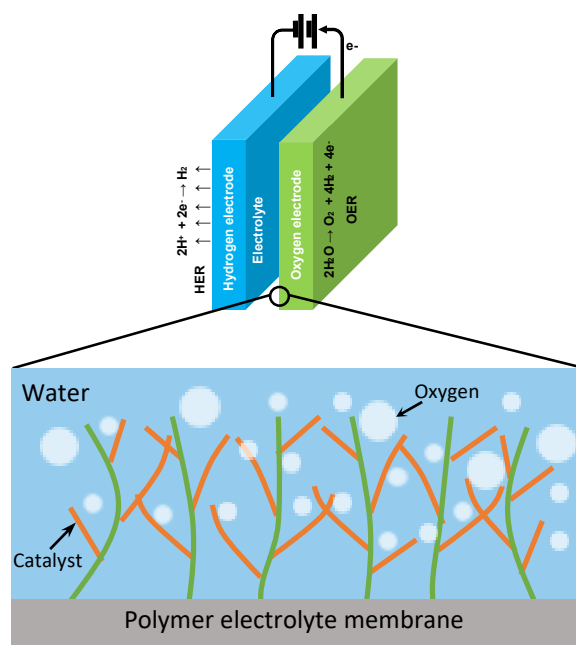
Shangfeng Du and Neil V Rees

University of Birmingham

Email: S.du@bham.ac.uk

Project description

The biggest challenge with current proton exchange membrane water electrolyzers (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 IrO₂- 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 IrO₂ and metal oxide materials.
- Surface deposition technique of SrIrO₃ on nanowire arrays.
- Electrode evaluation using both half-cell and single cell test.



Modified transition metal catalysts for hydrogen and oxygen evolution

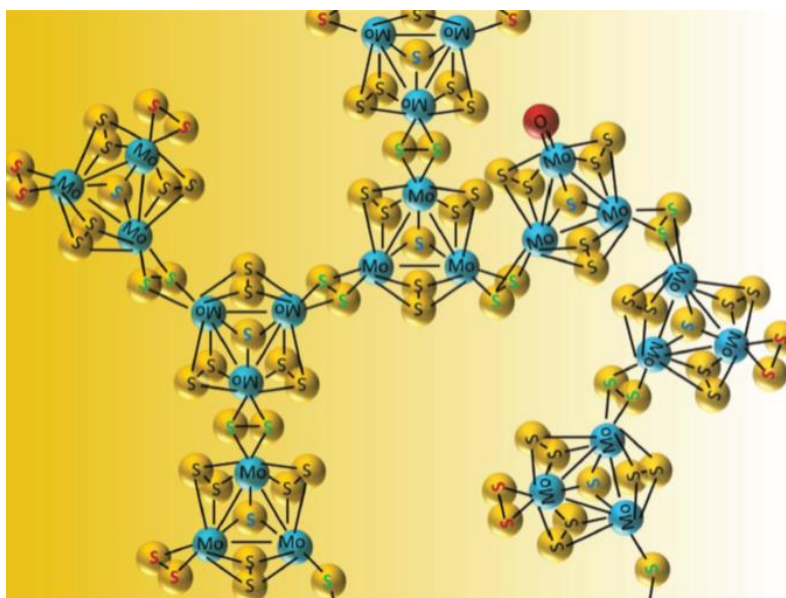
Neil V Rees and Shangfeng Du

University of Birmingham

Email: N.rees@bham.ac.uk

Project description

Transition metal dichalcogenides (TMDs, eg MoS₂, WS₂) 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



Business cases for Green Hydrogen

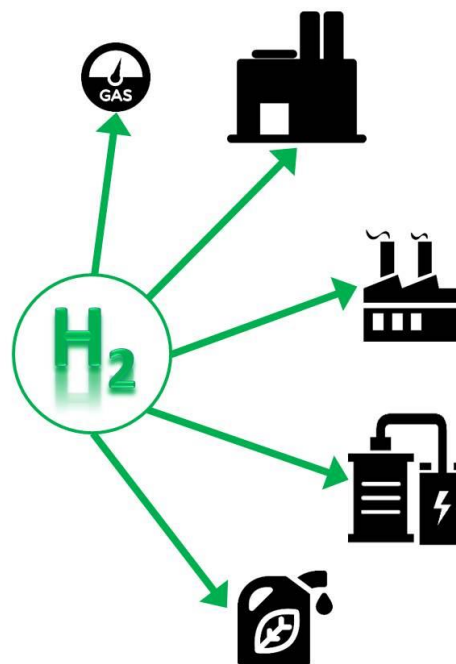
Robert Steinberger-Wilckens, Christoph Biehl and Jan Bebbington

University of Birmingham

Email: R.steinbergerwilckens@bham.ac.uk

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



The use of hydrogen as a processing gas to produce rare earth magnets

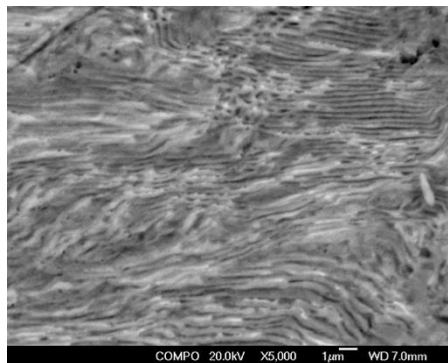
Allan Walton, Richard Sheridan and David Book

University of Birmingham

Email: A.walton@bham.ac.uk

Project description

Hydrogen is used in the conventional production of sintered (rare earth) neodymium-iron-boron magnets and in the recycling of these materials. The University of Birmingham has led international efforts in both of these areas. In recent years the Magnetic Materials Group have been developing new methods to manufacture rare earth magnets based on a process called hydrogen ductilisation. This process involves heating cast alloys in hydrogen to modify the microstructure. The material which is produced is ductile and can be shaped at room temperature. This reduces the number of process steps, reduces waste and could give a significant economic advantage to magnet manufacture. However the process is far from optimised and the aim of this project will be to develop this process alongside the team in Birmingham.



Deliverables

- An alloy system with complete ductility
- A matrix of hydrogen processing conditions for a range of alloy systems.
- 80% height reduction on pressing at room temperature
- Ultimately a netshape process route for magnet manufacture



Prevention and mitigation of incidents involving hydrogen use in a domestic setting

Sile Brennan, Donatella Cirrone and Vladimir Molkov

Ulster University

Email: sl.brennan@ulster.ac.uk

Project description

With a growing interest in the introduction of hydrogen to the natural gas grid, and its resultant use, including pure hydrogen, in homes for heating, cooking and power supply it is important to understand the specific hazards and associated risks pertinent to the use of hydrogen in a domestic setting. Appliances such as fuel cells, boilers, and burners, are being developed specifically for use with hydrogen and hydrogen blends. Validated contemporary CFD models and reduced engineering tools for reliable prediction of an incident dynamics in a residential setting are needed for reliable hydrogen safety engineering. Safety challenges include understanding the behaviour of a leak of hydrogen or hydrogen blends, including harmful impurities, validation of the similarity law for concentration decay in momentum-dominated jets for blends, application of the under-expanded jet theory to blends, assessment of leak and dispersion of flammable gas from flanges and joints, safety strategies to exclude accumulation of flammable mixtures, and appropriate venting strategies. The effect of buoyancy on the release of hydrogen blends could also be investigated. Hydrogen specific prevention and mitigation concepts are needed to efficiently tackle hydrogen dispersion and combustion in residential environments. There is a need to understand and exclude the potential thermal and pressure effects of an incident on the integrity of the property.

The expected impact of the study could include: validated contemporary CFD models and engineering tools for hydrogen safety engineering; deeper knowledge of the underlying physical phenomena; innovative prevention and mitigation strategies; guidelines for inherently safer design and use of hydrogen in a domestic setting, etc.

The study will focus on a combination of theoretical and numerical (CFD) studies, the use of ANSYS Fluent as a computational engine, multi-processor Linux-based hardware of HPC suite, etc. The results of this doctoral research will be aligned to HySAFER's externally funded projects and reported at international conferences as relevant. Publication of results in peer-reviewed journals is expected.



Deliverables

- Identification and prioritisation of relevant knowledge gaps.
- Theoretical and numerical studies to close knowledge gaps and address technological bottlenecks.
- Development of innovative safety strategies and engineering solutions to prevent and mitigate incidents with hydrogen and its blends in domestic settings.



Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

- Determination and characterisation of specific hazard and associated risks.
- Development and validation of novel engineering tools required for hazards and risk assessment.
- Evaluation of the effectiveness of conventional and innovative prevention and mitigation techniques and incident management strategies concerning specific hazards implied with the use of hydrogen or its blends in domestic settings, etc



Safety of using ammonia in for the hydrogen economy

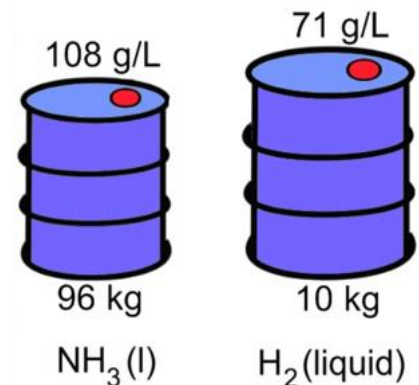
Dmitriy Makarov, Vladimir Molkov and Volodymyr Shentsov

Ulster University

Email: dv.makarov@ulster.ac.uk

Project description

There is a growing focus on hydrogen technologies and the role they likely to have in the development of the future low-carbon economy. The experience accumulated with use of ammonia in industries and its transportation around the globe offers practical, cost-effective means for storage and transport of large quantities of hydrogen compared to compressed gaseous or liquid forms. Ammonia is characterised by its liquid state at ambient conditions, high volumetric and gravimetric energy density. There is a substantial track record and experience on the inherently safer use of ammonia in the industrial environment as it is widely utilised in chemical processing, food production, as an agricultural fertiliser, etc. Emerging of ammonia in a different capacity, i.e. as hydrogen carrier, calls for a reassessment of hazards and associated risks it presents to life, property and environment. This PhD project aims to develop scientifically underpinned safety strategies and engineering solutions for handling large quantities of ammonia used as hydrogen carrier during transport and storage onboard and using relevant infrastructure. The project will review hazards, including toxicity effects, existing prevention and mitigation safety strategies when dealing safely with ammonia. New practices associated with extended use of ammonia for hydrogen economy will be investigated, scenarios of unscheduled ammonia release in enclosures and the open atmosphere will be identified and prioritised. The research outcomes are expected in the form of recommendations for inherently safer use of ammonia for hydrogen applications and may include, e.g. requirements to ventilation in enclosures where ammonia is handled, strategy for the choice of ammonia piping and pumping pressures, a methodology to define hazard distances for different release scenarios in the open atmosphere, others. It is envisaged that the research will rely on the use of Computational Fluid Dynamics (CFD) to study the propagation of ammonia cloud following its accidental discharge and evaporation, the build-up of ammonia concentration and its effect on exposed people. 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-processor workstations available at HySAFER Centre and HPC facility available within EPSRC KELVIN-2 project. This research will be aligned to HySAFER's





Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

externally funded projects and reported at international conferences. Publication of results in peer-reviewed journals is expected.

Deliverables

- Prioritised list of accident scenarios,
- Engineering model and/or CFD simulation problem formulation(s) for assessment of hazards in identified accident scenarios,
- Model implementation and completing simulations,
- Validation of the model(s) against available experimental data (or highly accurate solutions),
- Development of safety recommendations for handling ammonia as hydrogen carrier.



Modelling and simulation of premixed combustion in large-scale confined geometries

Dmitriy Makarov, Vladimir Molkov and Volodymyr Shentsov

Ulster University

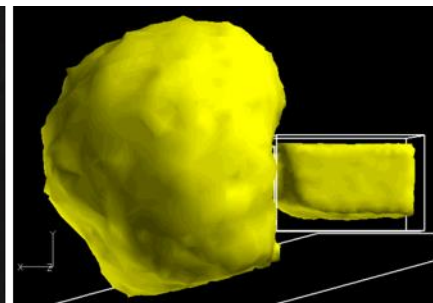
Email: dv.makarov@ulster.ac.uk

Project description

Pressure and thermal effects from large-scale deflagrations in large-scale confined geometries like a tunnel can be extremely hazardous due to the transition of initially laminar premixed combustion to the fast deflagration and potentially through the deflagration-to-detonation transition (DDT) to detonation. The role of various flame front instabilities and combustion acceleration mechanisms, especially in a confined and congested environment, is still not fully understood especially at large scales. Moreover, the interaction and thus the development of different instabilities and mechanisms on deflagration dynamics is not yet clarified. The Ulster's multi-phenomena deflagration model is under continuous development during last two decades in different parts of the globe. The model currently accounts for the dependence of burning velocity on changing during combustion pressure and temperature of the unburnt mixture, turbulence generated by flame front itself, turbulence in unburnt mixture, increase of burning rate due to preferential diffusion in stretched curved flamelets in the turbulent flame brush, fractal structure of turbulent flame front, etc. The model has been under continuous validation against a growing number of large-scale experiments, primarily hydrogen-air deflagrations, DDT and even detonations. It is expected that a candidate will develop the model further using the state-of-the-art in the field and expand the validation domain to the problems of practical importance including deflagrations of non-uniform hydrogen-air mixtures in tunnels or similar confined geometries. Experimental data on large-scale deflagrations are available for use as validation tests from ongoing projects, e.g. experiments on hydrogen release and deflagration in a large-scale tunnel at Health and Safety Executive test grounds within the H2020 HyTunnel-CS project, as well as previous projects in which Ulster University participated, partners in various European projects, and from literature. The successful candidate is expected to have a strong background in one of the following disciplines: physics, fluid dynamics, heat and mass transfer, combustion, computational fluid dynamics, safety engineering, etc. Any previous experience of analytical analysis and/or numerical modelling 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 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.



Explosion experiment



Explosion CFD simulation



Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

Deliverables

- Analytical and/or CFD model formulation and development
- Model(s) validation



Safety assessment and mitigation of hazards from TPRD in-situ of hydrogen vehicle

Dmitriy Makarov, Volodymyr Shentsov and Sergii Kashkarov

Ulster University

Email: dv.makarov@ulster.ac.uk

Project description

High-pressure hydrogen releases from thermally activated pressure relief device (TPRD), if ignited, can generate significant thermal and pressure loads on humans and structures. TPRD is required by regulation to exclude onboard hydrogen tank rupture in a fire by the release of hydrogen. The design and position of TPRD should be optimised to provide the shortest time of reaction to the fire and to allow passengers' rescue and self-evacuation in the case of accident without being compromised by hydrogen jet fire resulting from TPRD release.

This study aims to develop a comprehensive computational fluid dynamic (CFD) model for high-pressure hydrogen release and combustion from a realistic TPRD nozzle to aid safer design of TPRD for high-pressure hydrogen storage onboard vehicles. The research project will address the following design challenges:

- TPRD nozzle and pipeline design should provide for minimal possible flame length and associated hazard distances not to impede on passengers' self-evacuation and operation of rescue services.
 - In the same time the TPRD design should exclude flame blow-off during tank blowdown to avoid accumulation of hydrogen and formation of explosible hydrogen-air mixture.
 - Ignited or unignited hydrogen release from TPRD should exclude potential for development of the pressure peaking phenomenon (PPP) if initiated in a domestic garage or maintenance workshop.
- TPRD assembly performance should exclude its false initiation during fast hydrogen fueling

Research outcomes of this study are expected in the form of recommendations for safe design of TPRD for onboard hydrogen storage. The candidate will work alongside HySAFER team members contributing to development of regulations, codes and standards in the area of hydrogen fuelled vehicles safety. Strong background in one or more of the following disciplines is expected: mathematics, physics, chemistry, fluid dynamics, heat and mass transfer, combustion, computational fluid dynamics. Any previous experience of theoretical analysis and/or numerical studies is welcome. The PhD researcher 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 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.





Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

Deliverables

- Collection of information about TPRD and automobile fires
- CFD and/or CFD-FEM model formulation and development
- Validation of CFD and/or CFD-FEM model
- Parametric studies using CFD and/or CFD-FEM model
- Formulation of recommendations for TPRD design



Using coupled CFD-FEM modelling for the safety assessment of hydrogen-powered vehicles

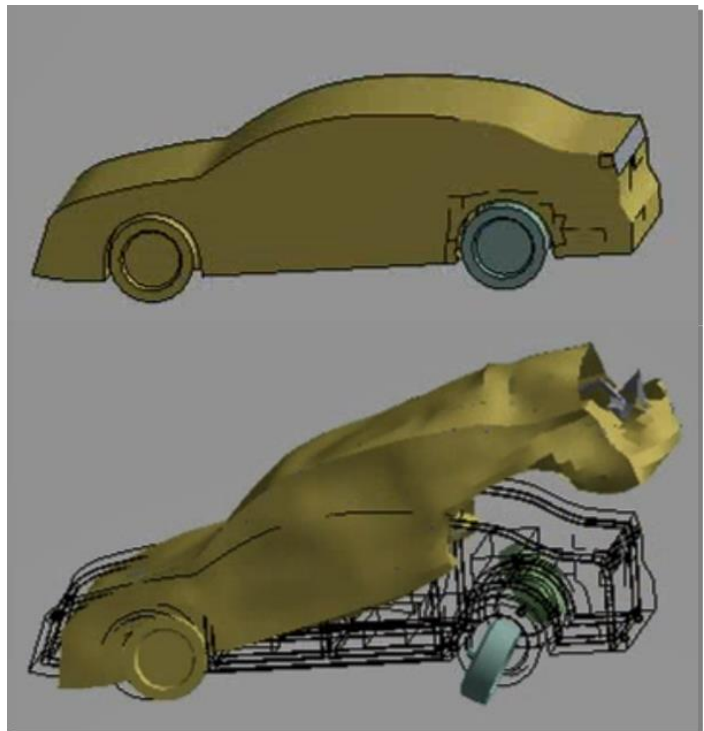
Volodymyr Shentsov, Dmitriy Makarov and Vladimir Molkov

Ulster University

Email: v.shentsov@ulster.ac.uk

Project description

Hydrogen-power vehicles are being parked in garages, maintenance shops, underground parking, tunnels and other confined spaces. Blast wave and fireball following the high-pressure tank rupture in a fire represent a major hazard threatening life and incurring property losses. Vehicle deformation and displacement after onboard hydrogen storage tank rupture consumes a part of mechanical energy of compressed hydrogen, affects hydrogen combustion and thus the contribution of chemical energy to the blast wave strength. The fireball dynamics is also affected by the presence of the vehicle. Hazards of under-vehicle tank rupture in the open atmosphere do not apply to confined scenarios, e.g. tunnels where the blast wave propagates with little decay compared to the open space and fireball propagates with large velocity for long distances compared to the open space. Assessment of energy to deform and displace vehicles is essential to develop engineering tools with a realistic prediction of pressure and thermal loads that would not be over-conservative. This energy can be assessed using the Finite Element Method (FEM) modelling and simulations. The project aims to develop a coupled CFD-FEM model applicable to the analysis of consequences of onboard hydrogen storage tank rupture in a range of conditions – tank volume, pressure, mounting position on a vehicle, vehicle location, etc. Computational tools for fluid flow simulations and structural analysis will be used as a platform for model development. Experimental data available in the literature and from HyTunnel-CS project will be used for the model validation. This doctoral study includes identification and prioritisation of knowledge gaps and technological bottlenecks; performing theoretical and numerical studies to close identified knowledge gaps; numerical analysis of structural response to thermal and pressure loads; quantitative assessment of pressure and thermal hazards and associated risks; development and validation of innovative engineering solutions and tools for hydrogen safety engineering, etc. The following aspects and phenomena will be considered: contribution of chemical energy of hydrogen combustion into the strength of the blast wave; blast wave and fireball effect on the structural elements of confined spaces; mitigation of the blast wave e.g. by tunnel splits, laybys, etc.; projectiles, including vehicle, and hazard distance assessment; reduction of projectiles hazards based on the tank location, etc. The expected





Sustainable Hydrogen

CENTRE FOR DOCTORAL TRAINING

outcomes of the study include: validated contemporary models; a deeper knowledge of the underlying physical phenomena; innovative prevention and mitigation strategies; etc. The successful candidate will work at HySAFER Centre and will focus on CFD-FEM modelling with use of relevant ANSYS software and Northern Ireland High Performance Computing (NI-HPC) Kelvin-2 cluster. The results of this doctoral research will be used in HySAFER's externally funded projects and will be reported at international conferences. Publication of results in peer-reviewed journals is expected.

Deliverables

- Problem formulation for the coupled CFD-FEM model
- Coupled CFD-FEM model implementation
- Validation of the coupled CFD-FEM model
- Formulation of recommendations for mitigation of the onboard tank rupture accidents