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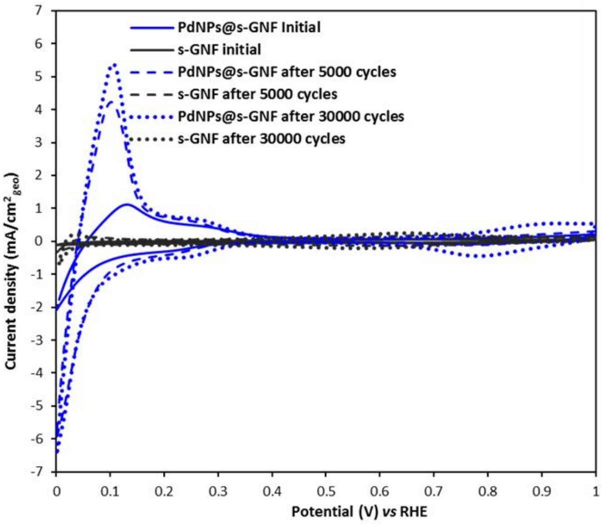
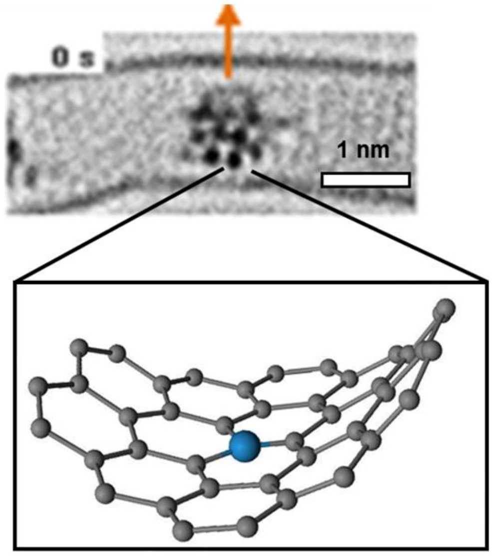
Electrocatalytically Active Carbon Nanoreactors for Hydrogen Production & Utilisation

Elena Besley, Jesum Alves Fernandes and Andrei Khlobystov
University of Nottingham
Email: Elena.Besley@nottingham.ac.uk

Project description

Nanoclusters of catalytically active transition metals (Pt, Pd, Ni) will be integrated with carbon nanotubes or hollow carbon nanofibers using computational predictions of the metal-carbon bonding and interactions. Guided by computational modelling, control of electrochemical activity will be achieved through fabrication of metal nanoclusters with bespoke size and composition, and by defect engineering (e.g. step-edge, vacancy) in the carbon nanoreactors. Electrochemical activity and durability of the electrocatalytic nanoreactors will be tested in the hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR), and structural / chemical changes in the electrocatalyst will be monitored at nanoscale by TEM, Raman and XPS. The computational modelling of HER and ORR will underpin the obtained results.





Deliverables

- New family of electrocatalytically active materials with potential applications in water electrolysers and / or fuel cells.
- Atomic scale understanding of the evolution of meta-carbon bonding during electrocatalytic reactions.
- Electrocatalytic activity and durability outperforming existing materials.

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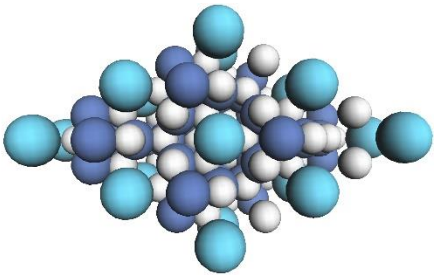
UKRI Engineering and Physical Sciences Research Council

Synthesis and characterisation of metal alloys for hydrogen storage and related applications

David Grant, Gavin Walker and Sanliang Ling
University of Nottingham
Email: David.Grant@nottingham.ac.uk

Project description

Decades of research have been devoted to storing hydrogen more economically and efficiently, and solid-state stores based on hydrides of metal alloys, such as intermetallics and high-entropy alloys, are one of the most extensively studied materials. A wide range of exciting potential applications are available, from hydrogen storage for transportation, stationary applications for refuelling and energy storage, to hydrogen compressors and thermal energy storage. Their practical applicability varies widely as a function of their thermodynamic properties which, when combined with other factors such as sustainability, cost, kinetics, capacity, has led to thousands of metal hydrides being investigated experimentally. Working together with an in-house modelling group, who will run computational high-throughput screening of materials databases and identify new candidate metal alloys with favourable properties for the aforementioned applications, this project aims to experimentally synthesize new metal alloys shortlisted by computational screening, and characterise their structures and hydrogen absorption/desorption properties. This project forms part of our ongoing collaboration with Sandia National Laboratories on a joint experimental/computational project to identify new metal alloys for hydrogen storage and related applications.



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Development of odour additives for use in H_2 technology

Marc C Kimber and Gareth J Pritchard
Loughborough University
Email: M.C.Kimber@lboro.ac.uk

Project description

A key challenge for the effective adoption of hydrogen technology is safety. There are significant safety risks in using and storing hydrogen; H2 is 14x lighter than air, it is odourless, it is colourless and importantly H2/air mixtures can readily ignite over significant distances. The rapid detection of H2 leaks is imperative to ensure that there is sufficient public confidence and that the technology becomes acceptable. Typically, hydrogen sensors are used to detect H2 leaks. This technology it is well established but would unsuitable for emerging hydrogen technology markets given their cost. Additionally, a method for sensing hydrogen leaks, either through smell (or sight) would beneficial in increasing public confidence in hydrogen technology.

Odour agents are typically unpleasant smelling organic compounds added to an odourless gas that when detected by the human nose provoke alarm. Natural gas is odourless, but we immediately recognise a leak from the smell of an odour agent added to the natural gas, tert-butylthiol. This signals an immediate alarm, as well as providing assurance that we can effectively sense the leak if required.

However, unlike natural gas, odour additives used for hydrogen use and storage has significant limitations. Firstly, typical aliphatic sulphur and nitrogen based odour agents can impact the catalysts used within fuel cells; and secondly, the odour agents must be non-toxic given the use of hydrogen gas in domestic markets.

This project will design and synthesize new odour additives for hydrogen storage, and then benchmark them against the current industry standard(s). Their will be three elements to this project (1) synthetic chemistry modification of the recently divulged sulphur and nitrogen free method using acrylate/acetophenone (antioxidant) system;(2) the development aromatic thiophene and derivatives, where their structures can be modified to reduce (or eliminate) catalyst poisoning in fuel cells; and (3) use of carbon rich saturated readily available natural products (e.g. longifolene). This latter element of the project goes against existing paradigms in odours additives, but we believe these substrates remain underutilised as potential odorants, particularly given they are aliphatic and contain limited functional groups that could potentially poison a catalyst with a fuel cell.

The implementation of the results from this project will provide novel odour agents that can be used in hydrogen storage. By delivering a cost-effective method for hydrogen detection, public confidence in hydrogen technology will be enhance. This should see an increased uptake of hydrogen technology by business, thereby reducing reliance on fossil fuel use leading to decarbonisation of the economy. Additionally, a more cost-effective safety platform should see hydrogen technology becoming more available to developing economies and emerging markets

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Deliverables

- Novel odour agents for use in hydrogen technology and storage.
- A methodology for accessing odour agent poisoning in hydrogen fuels.

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Lowering the H_2 cost in Methane Cracking Technology by use solid carbon as an Energy Storage Material.

Upul Wijayantha, Niladri Banerjee, Pritesh Hiralal (Zinergy UK)
Loughborough University
Email: U.Wijayantha@lboro.ac.uk

Project description

The Covid-19 lockdown provided us an invaluable opportunity to gather much needed real data to strongly argue for switching to a carbon emission free energy vector (eg. hydrogen) at earliest. As the world is now gradually moving to the *post-Covid 19 peak era*, by switching to hydrogen and renewable based energy system, we will be able to maintain the CO2 emission levels at that of the Covid-19 lockdown period. In fact, hydrogen could play a major role in all major areas of our energy landscape: namely domestic, transport and industry. However, for this transition to take place hydrogen has to successfully compete with current energy systems based on oil and gas resources. The economic case for it rests on two preconditions that complement each other; the first is that hydrogen can be produced affordably using environmental-friendly methods, and the second is that hydrogen utilization technologies will gain a significant market share in competition with other alternatives. In addition, technological advances in distributed hydrogen production would eliminate the stringent requirements in storage and transportation of hydrogen.

Thermochemical and electrolytic methods are leading the scaled hydrogen production today, however, the cost of production is still a major barrier which prevent its adaptation at scale. As far as affordable hydrogen production is concerned, alternative and flexible production methods such as methane cracking are rapidly picking up today.

Methane cracking which converts methane to hydrogen and capture carbon as a solid product, is a potential bridge technology during the transition to a sustainable hydrogen economy since it produces hydrogen with zero emissions of carbon dioxide. The process is flexible enough to alter the conditions to obtain value-added solid carbon (eg. single, double and multi-walled CNT, highly porous carbon). These solid carbon products are highly sought in many technology areas such as energy storage, air and water purification, food and beverage.

This project is designed to investigates systematic alteration of process conditions to obtain value-added solid carbon specifically for energy storage area whilst high yield of hydrogen is still maintained. By doing this we aim to obtain high value-added carbon products and high yield of hydrogen. The project team will work with the Cambridge based Zinergy UK to industrial bench marking the solid-carbon and evaluate its commercial potential. (Zinergy UK is working to deliver flexible energy storage solutions for a wide range of areas including healthcare, defence and smart and remote working areas).

Initially this project will recreate the current state-of-art hydrogen conversion levels and then analyse the resulting solid-carbon by-product to understand the growth process and its dependence on the growth substrate/catalysts. EffecTech Group (a UK based gas specialist company) will provide methane for the project and gas handling training. Then, the individual process conditions will be studied (eg. temperature, catalyst formulation, methane flow rate) to obtain a series of solid-carbon products at high H_2 generation yield. The carbon products will then be used in supercapacitor electrodes and evaluate the energy storage properties. Frequent sample exchange with Zinergy UK will ensure benchmarking and market value of solid carbon products that we will make.

The team will also maintain close links with other relevant UK industry to provide sample solid-carbon products to maximise their commercial potential in the short and medium term. The student who undertake this project will be able to gain skills in broad areas such as energy materials, hydrogen production and handling, catalysis, energy storage, supercapacitors etc and expose to the relevant UK industry. All above mentioned areas require skilled work force in the UK.
Student will also interact with another student based in School of Business and Economics who will develop business models for adaptation of methane cracking technology.

Deliverables

- Generate H_2 at high yield whilst preparing value-added carbon for energy storage (eg. supercapacitors).
- Benchmarking performance of carbon products in energy storage and evaluate the commercial potential (in line with business models) in collaboration with industry.

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Metal membranes for separating pure hydrogen from gas grids

David Book, Shahrouz Nayebossadri, 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 (CH_4/H_2 and H_2 grids)

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Modified transition metal catalysts for hydrogen and oxygen evolution

Neil V Rees, 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.

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Development of high-performance complex hydrides

Daniel Reed, David Book
University of Birmingham
Email: d.reed@bham.ac.uk

Project description

Hydrogen is a promising low-carbon energy vector. However, many applications will require storage solutions with higher performance properties, such as improved gravimetric energy density volumetric energy density, thermal conductivity, electrical conductivity, and/or reversibility (i.e. cycling stability).

In this project, boron-based and nitrogen-based complex hydrides will be synthesized by chemical and mechanochemical routes (or sourced) and their hydrogen storage, electrical, and thermal properties will be assessed in detail.

In particular, a powerful and versatile Raman spectroscopy technique will be utlizied. It is sensitive to both crystalline and amorphous materials, and able to follow a reaction across a change of state, from solid to liquid or liquid to gas (and vice versa). Raman spectroscopic measurement and analysis techniques will be carried out. A Raman microscope with in situ cells capable of performing variable temperature (-180°C to 1500°C), variable pressure (vacuum-100bar), calorimetric and electrochemical measurements has been developed.

Deliverables

- Development of complex hydrides with improved hydrogen storage properties
- Find new, crossover applications that ultilize novel electrical, thermal and magnetic properties of families of boron- and nitrogen-based complex hydrides
- In situ Raman techniques for characterization of complex hydrides

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Algal Biomass to Hydrogen: A Circular Approach for Green Sustainable Processing with Enhanced Efficiency and Minimal Waste

Bushra Al-Duri, Rafael Orozco, John Love, Lynn Macaskie,
University of Birmingham
Email:b.al-duri@bham.ac.uk

Project description

The project investigates hydrothermal conversion of algal biomass to H_2-rich gas in a sustainable circular approach. Figure 1 is a conceptual diagram of the technology pathway in general: Cultivated wet microalgae (MA) undergoes hydrothermal liquefaction (HTL) in subcritical water, and the products are separated into gases, oil phase (biocrude), and aqueous phase (organics-rich). The biocrude oil can be catalytically hydrotreated to hydrocarbon fuels, and the organics-rich aqueous phase undergoes gasification in supercritical water conditions to produce H_2-rich gas. The HTL process is the gateway to paths (1) and (2). HTL conditions (specifically reaction time, temperature) dictate the products' composition, and product separation technique influences the products' distribution between the aqueous and oil phases**.** Also, they influence the %H_2 in the gas exit stream. **This project investigates MA cultivation followed by the optimum conditions that favour an aqueous phase rich with organic matter -path (2)-, where organics undergo SCWG to produce H_2 gas.**

Why SCWG? a) SCWG is the only advanced hydrothermal technology known to convert the entirety of organic matter to H_2-rich gas *without the concurrent generation of chars and tars*. b) SCW indiscriminately dissolves all organics which makes SCWG a one-phase reaction with minimal diffusion limitations and very high rate, c) the aqueous phase after SCWG would be rich with nutrients that can be recycled for algal growth, c) SCWG is ideal for wet biomass thus no drying is required, d) the hot exit gas from SCWG contains high-grade heat, which can be integrated to enhance the process exergy efficiency.

Figure 1 offers flexibility to reach the desired product(s) based on the microalgae (feedstock) composition and process conditions. The criteria would be product purity, quantity, waste minimisation (towards circular economy), energy integration and economic feasibility. After investigation of HTL parameters the project workers will establish the best route to achieve the above-mentioned criteria. The project involves a focused experimental programme, feedstock and products analysis, theoretical investigations and simulation for best energy integration scenario, and of economic feasibility. We plan to focus on the existing technology barriers namely (i) efficient oil/water separation seeking organics-rich aqueous phase, (ii) optimum SCW gasifier design, (iii) maximum energy recovery and integration (via simulation), and (iv) maximum H_2 production. This programme is a start of more detailed and rigorous programme for an efficient & economically feasible H_2 production plant with zero waste.

Why microalgae? Use of microalgae offers significant advantages such as: sustainable supply (can be cultivated throughout the year and in most climates), fast growth rate, maximum biomass production, relatively high photosynthetic efficiency, minimum pre-treatment (maceration), no use of arable land and CO_2 capture & storage-a carbon neutral process for energy from sunlight. In general, algae biomass contains 20-30% carbohydrate, 10-20% lipid, and 40-60% protein. The ratio of the algae's composition fractions influences the effect of catalysts (K_2CO_3 or NaOH) and gasification products; of particular interest for this project is the protein fraction in microalgae, as it known to have adverse effects on gasification efficiencies, hydrogen generation and catalyst performance. Hence a key work package will be to study and understand these interactions. In the cultivation process; researchers have been able to manipulate microalgae growth conditions to favour a particular fraction (For example, under nitrogen limitation, microalgae tend to produce more lipid than carbohydrate and protein).The challenge of minimising protein fraction is another key goal of the project.

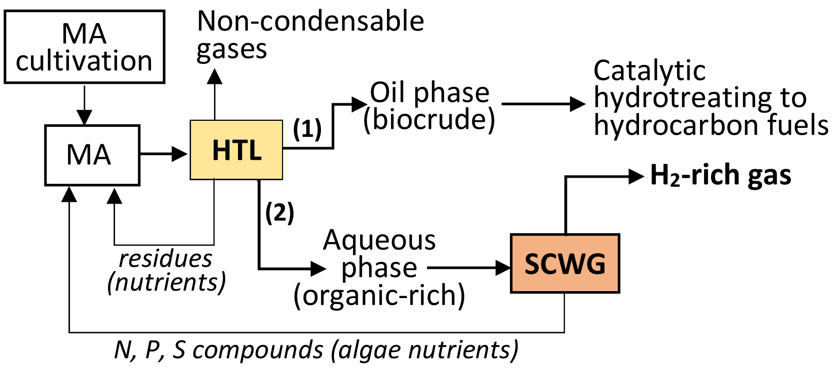

Figure 1. Conceptual diagram of the Process

Deliverables

- Designed HTL unit with flexibility of path towards desired final product(s).
- Designed SCWG unit to maximise H_2 production and recovery.
- Fully designed, energy integrated continuous process to convert feedstock microalgal biomass to H_2-rich gas, with maximum efficiency and minimal waste.
- At least 2 scientific publications and presentation of work in at least 2 relevant international conferences.

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Robust proton exchange membrane water electrolysers with thin film nanostructured electrodes

Shangfeng Du, Neil V Rees and Anthony Kucernak
University of Birmingham
Email: S.du@bham.ac.uk

Project description

The biggest challenge with current proton exchange membrane water electrolysers (PEMWE) is their poor durability, which is mainly caused by the degradation of the electrode structure under high operating pressure and humidity in long-term operation. The loose electrode structure from catalyst nanoparticles cannot stand their robust long under the severe condition in PEMWEs. In this PhD project, we'll develop a new generation of electrodes by growing aligned IrO2-based nanowires directly on polymer electrolyte membrane to develop highly robust thin film electrodes for PEMWE applications. The new electrode structure will provide (i) high electrode durability from a boosted strong contact between the nanowire catalysts with electrolyte membrane, (ii) enhanced catalyst stability from the low degradation rate of one-dimensional nanowires compared to 0-dimensional nanoparticles, and (iii) improved power performance resulting from the significantly reduced mass transfer losses from the unique thin catalyst layer together with the open electrode structure of and aligned nanowires. It's expected to achieve >50 mV decrease in electrolyser overpotential at 1 A cm^{-2} compared to commercially electrode system (i.e. 4% efficiency improvement).

Deliverables

- Month12: Complete all modules required, finish the literature research.
- Month 18: Modify the substrate surface to get uniform nanowire grown.
- Month 30: Successfully grow IrO2 based nanowires on substrate. Publish one paper on international reviewing journal, present the results at one international conference.
- Month 42: Confirm the feasibility for the deposition of $SrLrO_3$ on IrO_2 based nanowires.