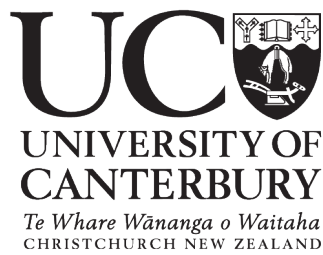


New Zealand Hydrogen Symposium

2024 III I I

Book of Abstracts

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2024



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Solar Harvesting through Catalysis to Make Chemical and Fuel

Rose Amal

School of Chemical Engineering, UNSW

Turning to the Sun as an energy source to generate H_2 and its derivatives (such as ammonia, green chemical feedstocks and fuels) is an obvious place to focus our investigations because it reduces our reliance on unsustainable fossil fuels. There are a number of means in utilising the sun's energy to drive energetically demanding catalytic processes. We can use (i) electricity from photovoltaic transformation of sunlight to drive electro-catalytic reactions (electrocatalysis), (ii) heat of the sun to activate thermal catalyst (thermal catalysis), and (iii) light of the sun to excite electrons from valence band of a semiconductor to its conduction band (photo catalysis).

Here, I present our ongoing research in harnessing the full solar energy spectrum (from ultraviolet to infra-red) to induce or/and enhance catalytic water splitting or photoreforming to generate H_2 , to reduce CO_2 and H_2O to make Syngas ($CO + H_2$), and drive NO_x reduction reactions to produce ammonia.

In electrocatalysis, our approach involves making electrodes more cost-effective by reducing the reliance on precious metals like Pt, either by lowering their required amounts or substituting them with more economical catalysts such as Ni, Fe, Co, and Carbon. As the energy transition underscores the importance of minimising mineral loading, two strategies are employed: first, increasing the number of active sites, often achieved by downsizing catalysts to single-atom or cluster levels, and second, tuning intrinsic properties of these active sites. Intrinsic tuning involves doping heteroatoms (e.g., Nitrogen, Phosphorous), incorporating multi-elements (e.g., coupling Fe and Cu), and altering the coordination environment through vacancy engineering and defect creation. These strategies enhance the activity of active sites and provide better control over their selectivity.

Determining the relationship between physical degradation and voltage decay of a proton exchange membrane electrolyser

Samuel Jack Clarke*, Thea Larsen, Andrea Kolb, Seho Kim, **Jingjing Liu***

Department of Chemical and Materials Engineering, The University of Auckland

This research project focuses on the efficient control and degradation mechanisms of a Proton Exchange Membrane (PEM) electrolyser. Degradation and performance issues associated with PEM electrolysers require amending to reduce costs and increase hydrogen uptake from renewable sources.

The efficiency of PEM electrolysers was investigated to understand the effects of increased operating temperatures and current overshoots. Experimental work allowed the observation of an efficiency increase in the form of reduced input power consumption following increased operating temperatures and current overshoots.

These findings were significant in determining optimal operating conditions for PEM electrolysers. The two-year operational life has also led to voltage decay and reduced efficiency. The investigation of component degradation led to an explanation for voltage decay.

Additionally, the degradation of the Membrane Exchange Assembly and passivation of titanium components confirms the material degradation responsible for a voltage decay observed over the electrolyser's lifespan.

These findings confirm similar research and point out the regions that require improvement for effective long-term PEM electrolysis functionality.

Australia's Hydrogen Industry Journey

Patrick G. Hartley

CSIRO Hydrogen Industry Mission

Australia's first National Hydrogen Strategy was developed and adopted by Australia's state, territory and federal governments in November 2019. Since then, industry and governments have together invested several billion dollars in delivering a broad suite of hydrogen industry projects across the nation.

CSIRO, Australia's National Science Agency, launched its Hydrogen Industry Mission in May 2021, with the goal of supporting global decarbonisation by enabling a commercially viable Australian hydrogen industry comprising both domestic and export value chains by 2030. The mission is actively supporting the development of Australia's hydrogen industry through a range of activities. These include industry and research knowledge sharing, strategic analysis, and delivery of a broad suite of research, development and demonstration projects. This presentation will offer perspectives on Australia's hydrogen industry progress so far, the role of research and development, and showcase recent highlights from CSIRO's Hydrogen Industry Mission.

Advanced Functional Nanoporous Materials for Clean Energy Technologies

Ajayan Vinu

Global Innovative Center for Advanced Nanomaterials, School of Engineering, The University of Newcastle

Nanoporous Materials with ordered porous structures and functional elements offer excellent textural features and catalytic properties. Among the nanoporous materials, nanoporous carbon nitrides are quite unique as they possess highly stable semiconducting CN framework with tunable band gaps and basicity.

These CN nanomaterials can deliver successful energy and environment solutions - such as converting waste or seawater into clean hydrogen with only sunlight and developing innovative devices for energy storage and conversion.

In this talk, I will present the development, capabilities, and current and future applications of multifunctional amorphous and crystalline nanoporous carbon nitride materials with different structures, band gaps, and nitrogen contents.¹⁻⁹ Especially, I will focus on the preparation of novel nanoporous amorphous and crystalline C_3N_5 , C_3N_6 , C_3N_7 and C_3N_8 materials and their structural elucidation using different spectroscopic techniques.

I will also demonstrate how the chemical composition, structure, porosity and the functionalization of these unique materials can be tuned, as well as the fabrication of nanoporous CN hybrids with single molecular precursors with C, N, S elements and with mono and bimetallic sulphides. In the last part of the talk,

I will present on the energy storage and photocatalytic performance of these unique nanoporous carbon nitrides and their hybrids on water splitting to produce clean hydrogen from seawater. I will also demonstrate the utilization of this technology on converting the seawater from different beaches along the coastal side of Australia.

1. Vinu et al., *Chem. Soc. Rev.* 2023, *In press*
2. Vinu et al., *Adv. Mater.* 2023, *In press*.
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Self-repairing anode catalysts for alkaline water electrolysis powered by renewable energy

Yoshiyuki Kuroda

Graduate School of Engineering Science, Yokohama National University

Water electrolysis is a key technology to produce H₂ from renewable energy.

Because proton exchange membrane water electrolyzers require noble metals as catalysts, alkaline-type electrolyzers, such as alkaline water electrolyzers (AWE) and anion exchange membrane water electrolysis (AEMWE), have attracted much attention for the use of nonnoble-metal-based catalysts.

One of the most important issues of AWE is the degradation of catalysts due to generation of reverse current upon shutdown and power fluctuation. Reverse current hardly generates in AEMWE in principle; however, it possibly generates if an electrolyte is supplied instead of pure water.

To overcome this problem, we propose self-repairing catalysts for oxygen evolution reaction of water electrolysis.

A self-repairing catalyst is dispersed in the electrolyte and deposited on the anode during electrolysis. If the deposited catalyst layer degrades under fluctuating power, the catalyst layer is repaired by the additional deposition of catalyst.

In this study, I will demonstrate that a hybrid cobalt hydroxide nanosheet, consisting of a cobalt hydroxide layer modified with organic molecules, acts as a good self-repairing anode catalyst under power fluctuations.

These insights will contribute to the development of novel electrocatalysts with high durability and high activity.

Hydrogen perspective in Japan

Mr Ohira Eiji

Advanced Battery & Hydrogen Technology Department, NEDO (The New Energy & Industrial Technology Development Organization)

Japan's bold vision for a hydrogen energy and carbon-neutral future is evident. Initiated in 2017 and recently revised, the Government of Japan's Basic Hydrogen Strategy is ambitious, with specific goals and strategies focusing on cost reduction and early implementation in sectors like transport and residential fuel cells.

Despite challenges, Japan's commitment to technological development, infrastructure, and international partnerships underscores its dedication to a low-carbon hydrogen energy system.

For further context and detailed insights into this strategy, Ohira-san has referenced two presentations: one from NEDO www.nedo.go.jp/content/100956596.pdf and another from IGES www.iges.or.jp/sites/default/files/inline-files/3-2_Eiji_Ohira_20230823_IGES.pdf. These documents provide an in-depth look at the ongoing research and development efforts supporting this initiative.

A Critical Analysis of Using an In-Situ Reference Electrode to Decouple Anode-Cathode Dynamics in an Anion Exchange Membrane Water Electrolyser

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¹University of Canterbury

²MacDiarmid Institute for Advanced Materials and Nanotechnology

This experimental study investigates the intricate behaviour of an anion exchange membrane water electrolyser (AEMWE) by decoupling the individual contributions of the anode and cathode. AEMWEs have garnered significant attention as promising devices for sustainable hydrogen production due to their inherent advantages, including enhanced cost-effectiveness compared to traditional proton exchange membrane electrolyzers. However, a nuanced understanding of the distinct electrochemical processes occurring at the anode and cathode interfaces is crucial for optimising their performance.

Impedance measurements of the whole cell often mask specific electrochemical processes occurring at each electrode. By isolating the anode and cathode, impedance measurements give insights into the electrochemical reactions, charge transfer processes, and related phenomena specific to each electrode. This decoupling allows for a deeper understanding of underlying mechanisms, improved analysis of performance limitations, and targeted optimization of individual electrode behaviour. Such advancements facilitate the refinement of electrochemical cell design and operation, benefiting fields such as energy conversion, electrochemical synthesis, and electroanalytical techniques.

One way to isolate electrochemical processes at a given electrode is to integrate a reference electrode into the cell. However, the location of the reference electrode can influence the results obtained. In an ideal scenario where the anode remains constant across multiple experiments, one might anticipate identical outcomes when comparing data from experiments where the reference electrode is positioned at the anode versus the cathode. The expectation is that, when the obtained data with the reference electrode on the cathode is corrected for ohmic influences to eliminate membrane effects, the results should mirror those obtained when the reference electrode is situated on the anode. However, this is not the case. This work investigates the advantages and limitations of using an in-situ reference electrode in AEMWE for impedance spectroscopy and polarisation studies.

A Practical Demonstration of Hydrogen Supplementing a Standalone Renewable Energy System

Holt R¹

¹Callaghan Innovation

Base Power an innovative New Zealand power company saw a demonstration of Callaghan Innovation's HyLink System at Gracefield Innovation Quarter. They were inspired to ask for a variation of the system to operate with their standalone power system (SAPS).

The project goal was to investigate how hydrogen can provide additional energy storage to a lithium battery stack.

Analysis of field data showed how much hydrogen might be captured and used to generate electricity on cloudy days.

Callaghan Innovation designed an alternative of the usual HyLink Electrolyser to operate as a variable load. The electrolyser operates as a flexible load to consume surplus solar power when it is available; after meeting consumer needs and filling the battery pack.

H2X in Taranaki designed and built a system to compress the hydrogen to 150barg. Compression permits the system to be compact enough to be deployed as per the original standalone power system. The total energy storage of the system increased 6-fold.

Electricity is generated from the hydrogen by mixing it into the air intake of an 11kW diesel generator, supplied by TerraCat in Christchurch. An elegant injection system enables the generator to operate without any modification to the diesel system, so if hydrogen is not available the SAPS operates as normal.

Several novel elements have been combined to investigate how effective hydrogen will be as an energy vector and method for GHG reductions, without compromise to the end user experience of a SAPS.

This work is a collaboration led by BasePower and supported by several businesses across Aotearoa New Zealand, with some valuable assistance from Queensland.

An Overview of the Hydrogen Storage Research Group (HSRG) at Curtin University

Buckley, C¹

¹Physics and Astronomy Curtin University

The HSRG under the leadership of John Curtin Distinguished Professor Craig Buckley has been conducting research on energy storage at Curtin University over the past 20 years. Over this period the HSRG has predominantly been involved in researching hydrogen storage materials, as well as heat storage materials and batteries. The 4 main areas of research are hydrogen storage for mobile and stationary applications, thermal batteries made from metal hydrides and metal carbonates, solid state hydrogen storage materials for export applications and solid state electrolytes. A selection of recent publications from the HSRG are given below^[1 – 9].

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Biohydrogen and biomethane production from soluble wood sugars

Wijeyekoon S¹, Ranganathan S¹, Vaidya A¹

¹Scion

Biohydrogen can be produced from biogenic carbon sources employing low-energy intensive biological processes. An estimated 4.4 million wet tonnes of waste woody biomass is produced in NZ that has a theoretical hydrogen production potential of 0.3 million tonnes. Key challenges to the realisation of this potential are the collection of the distributed resource and the higher energy required for gasification. Although wood contains bio-recalcitrant constituent such as lignin, the cellulose and the hemicellulose fractions of wood can be utilised to produce hydrogen and other co-products. In this study, we demonstrate biohydrogen and biomethane production from New Zealand's largest bioresource, the woody biomass. Debarked wood chips were steamed and screw pressed in a heated press to extract a liquid containing wood sugars. This solution was filtered and chemically characterised before reconstituting to feed into two separate bench-scale continuous bioreactors conditioned to produce hydrogen and methane by dark fermentation and anaerobic digestion. The gases produced were analysed for its composition by gas chromatography and the digestate for volatile fatty acids and residual carbon.

A biogas containing 20% - 40% hydrogen was continuously produced by dark fermentation. Nearly 30 L of hydrogen was produced over three hydraulic retention times (15 days) with a yield of 170 mL/g VS of feed. Acetate was the dominant volatile fatty acid produced indicating a metabolic pathway producing the highest hydrogen yield from sugars although other VFAs were also present in significant proportions. The biomethane yield from the same feed was 292 mL/g VS. On a volumetric gross calorific value basis, the hydrogen gas produced close to 19% of the energy produced by methane. The sequential hydrogen and methane production could improve the total energy yield from wood sugars and the combustion properties of the mixed gas.

Bio-inspired catalyst design strategy for green hydrogen production

Ghorai S¹

¹IIT Bombay

Production of green hydrogen from water electrolysis using renewable energy sources will be a key enabler in the global transition towards a carbon-neutral energy framework.¹ In nature, hydrogenase enzymes reduce protons from water at a very low overpotential values while operating at high turnover rates. An array of synthetic catalysts have been design by following the footsteps of hydrogenase architecture.² In this regard, an axial N-heterocycle-ligated cobaloxime core (Co-N₅) provides an excellent platform for the development of a model catalyst for HER. The poor solubility and instability of such cobaloxime derivatives in acidic aqueous medium limit its industrial application. Later on, these limitations were overcome with the rational incorporation of peripheral protic functionalities surrounding the cobaloxime core that imitates the enzymatic outer coordination sphere.

In this work, we have strategically incorporated small amines, amino acids, vitamins, neurotransmitters (dopamine), drug molecules (isoniazide), and even nucleic bases to generate a pool of artificial outer coordinating sphere mimics surrounding the cobaloxime core. This has led to the generation of new genres of active H₂ production catalysts with boosted photo- and electrocatalytic H₂ evolution properties with an improved aqueous and air-stability.³ Among them, the nucleic base appended complexes are found to be the leading H₂ production catalyst with turnover frequencies of ~12700 s⁻¹ and overpotential around ~400 mV.^{4,5} Hence, this demonstrates the importance of bio-inspired catalyst design strategy for effective HER in aqueous conditions. Moreover, this unique enzyme-inspired catalyst design strategy can be heterogenized in electrolyzers for industrial green hydrogen production.

Reference:

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Biomimetic catalyst design strategy for sustainable green H₂ production

Dutta A¹

¹IIT Bombay

The current global energy demand is primarily satisfied by carbonaceous fossil fuels (coal, oil, natural gas), which invariably emit a copious amount of CO₂, leading to adverse climate change effects. Renewable energy resources (solar, wind, tidal, etc.) have emerged as apt alternatives to resolve this conundrum; however, they require a stable energy vector due to their intrinsic intermittence. Hydrogen molecule fits the bill as it can be directly used in a fuel cell for energy production following a greener pathway.

Therefore, hydrogen production has become a bustling research area via sustainable methods. Since water is an abundant resource of protons and covers over 71% of the planet, hydrogen evolution from water via electrolysis is regarded as the future of our energy landscape. Our group has developed a strategy for designing synthetic catalysts based on the architectural framework of enzyme active sites.

The inclusion of proton exchanging outer coordination sphere (OCS) feature is found to be a key component for enhancing the catalytic performance for an otherwise weak catalyst core. This outer coordination sphere feature can be incorporated in the form of amino acids, vitamins, neurotransmitters, drug molecules, and even nucleic bases. The evolution of this unique genre of bio-inspired catalysts and its optimized application for electrochemical and photochemical H₂ evolution will be discussed in this presentation.

Boosting Electrochemical CO₂ Reduction in MOFs via Enhancement of Mass and Charge Transport

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Elevated atmospheric levels of carbon dioxide (CO₂), resulting from fossil fuel combustion and industrial operations, stand as a significant factor of climate change. Ongoing research utilising electrochemical methods aims to decrease atmospheric levels of CO₂ through electrocatalytic reduction into practical products. Metal-organic frameworks (MOFs) serve as promising electrocatalysts in regard to CO₂ reduction owing to exceptional surface areas and high modularity.

The potential of MOF electrocatalysts have not been fully recognised due to mass transport and charge transport limitations. Mass transport limitations arise from the poor solubility of CO₂ in aqueous conditions which may be solved utilising a gas diffusion electrode. Charge transport limitations arise from innate insulating properties of the MOF which may be solved by introducing conducting species within the pores. This research aims to fill the knowledge gap surrounding MOF electrocatalysts for CO₂ reduction in determining effective methods to overcome current limitations.

Can Hydrogen be Economically Feasible in Decarbonising Australian Steelmaking?

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Decarbonising the steel industry poses a significant challenge due to its status as a hard-to-abate sector. With the global steelmaking sector relying heavily on fossil fuels and contributing to 7% of worldwide emissions, decarbonising steelwork is a formidable yet critical task. Hydrogen has often been acknowledged as a promising energy source with the potential to produce no harmful pollutants, yet its large-scale integration in industry remains a complex task. Australia, being one of the largest green hydrogen producers, could potentially benefit from using hydrogen as an energy carrier in its steel production. However, there exist challenges associated with hydrogen storage, transportation, and handling. In addition, the crucial concern of economic viability must be addressed. The lack of comprehensive research has made it difficult to anticipate the adoption of hydrogen for steel industry. This study aims to evaluate the practical options for implementing hydrogen technology in Australian steel production. The study demonstrates the feasibility of using hydrogen and hydrogen carriers through various adaptable scenarios using a techno-economic analysis method.

Carbon emissions of exporting hydrogen and ammonia from New Zealand to Japan

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Endowed with a rich resource of renewable energy, Aotearoa has an opportunity to export low-carbon energy carriers, namely hydrogen and ammonia, to countries that are aiming for net zero carbon emissions. Accurate assessment of the greenhouse gas emissions involved in producing these energy carriers is necessary to verify that climate benefits are achieved.

We carried out a life cycle assessment of hydrogen and ammonia production in New Zealand for export to Japan to fuel electricity generation. The study encompassed production of hydrogen by electrolysis in New Zealand, conversion to ammonia (where applicable), liquefaction, transport to Japan and combustion in a thermal power station.

Under present conditions the emissions for both hydrogen and ammonia come to 0.71 kg CO₂eq per kWh_e of electricity produced in Japan. This is considerably higher than the carbon intensity of Japan's currently electricity grid, which is 0.46 kg CO₂eq per kWh_e, implying that there is no carbon mitigation achieved by using imported energy carriers for electricity generation. The emissions were mainly from the supply of the large quantity of electricity required for production of hydrogen in Aotearoa. For every 1 kWh_e produced in Japan, 5.1 kWh_e were consumed in New Zealand due to energy losses in the supply chain.

Considering these findings, Aotearoa must achieve a high level of decarbonization before producing hydrogen or ammonia so that genuine carbon savings can be realised.

Catalytic hydrogen elimination technology and research progress of catalysts for hydrogen combustion

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Hydrogen energy is one of the most promising clean energy sources in the 21st century. The development and application of hydrogen energy in the power generation, automotive, and energy storage industries are expected to solve the problem of energy waste and pollution effectively. However, due to the inherent characteristics of hydrogen, it is difficult to maintain high safety during production, transportation, storage, and utilization.

Therefore, hydrogen safety issues have become one of the main bottlenecks restricting the development of hydrogen energy. Catalytic hydrogen combustion is the method that can control hydrogen concentration quickly and effectively to eliminate hydrogen safety hazards. Usually, under atmospheric pressure conditions, when the hydrogen concentration in the environment is higher than 2.0 vol%, hydrogen removal reaction can be initiated spontaneously without additional energy supplied by mankind.

Catalytic hydrogen combustion is considered as one of promising technology, and compared to traditional hydrogen air combustion, catalytic hydrogen combustion has higher safety and efficiency, and water was the only byproduct which was generated. Among them, catalysts are the core of the catalytic combustion system, which have a significant impact on hydrogen conversion and reaction rate. Noble metal catalysts are composed of the supports and active components.

Due to the maximum activity of Pt and Pd in the catalytic hydrogen combustion process, catalysts with Pt or Pd are most common as active metal components. A large amount of research has been studied on Pt or Pd loaded on different types of supports. Although many material carriers for catalytic hydrogen elimination have been studied, there are still some problems, such as low thermal conductivity, high cost, degradation at high temperatures, and aggregation of noble metal active components in support materials. Therefore, there is still necessary to develop a type of catalysts with high catalytic activity and long durability.

Challenges and Opportunities for Green Hydrogen Production from Water Electrolysis

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Hydrogen holds the promise as green energy carriers for global scale storage of renewable energy, e.g., solar and wind, enabling the continuous usage of these diffusive and intermittent energy sources when used together with fuel cells. Water electrolyser is a cornerstone technology for the hydrogen economy, which requests highly efficient, low cost, and robust catalyst materials to reduce its current levels of energy consumption and cost. However, currently there is a gap between lab-scale research and industrial scale water electrolysis, effectuated by catalysts, cell design, and operation conditions.

This talk highlights the current challenges and opportunities for water electrolysis from a material perspective and showcases our efforts in developing electrocatalysts for oxygen evolution reactions (OER) and hydrogen evolution reactions (HER) in alkaline and acid electrolytes, as well as operando methodologies for understanding the catalytic processes and gas bubble behaviours. The commercialisation of some our work for water electrolyser industry also will be introduced to highlight the significance of material design from atomic to macroscopic to industrial scale.

Computational design of metal hydrides for hydrogen storage: From quantum effects to multi-scale simulations and machine learning

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Hydrogen storage in metal hydrides is the ideal solution for many systems where medium- to long-term storage is needed, as is the case for back-up power generators and seasonal energy storage, or when safety is a concern. Even though some companies already successfully sell storage systems based on metal hydrides, materials scientist are still searching for the ideal material that combines a high storage density at near-ambient conditions with fast reaction kinetics, a reasonable price, and low environmental impact. Computational modelling is indispensable on this quest, because it can deliver insights into hydrogenation processes that help to understand experimental findings and it can make predictions without the need to actually synthesize the material.

This contribution gives an overview of the wide range of computational methods that we employ to understand and predict the properties of metal hydrides for hydrogen storage. On the atomic scale, quantum effects from electrons and nuclei govern the material properties. They are calculated with ab-initio methods to investigate the structure, stability, and mechanical properties of hydrogen storage materials as well as the energy barriers during hydrogenation. Making relevant predictions for larger scales, however, requires integrating the results from the atomic scale into thermodynamic models and meso-scale simulations, such as phase-field models. While thermodynamics enable the prediction of the stable phases under given conditions, meso-scale simulations provide insights into the hydrogenation kinetics. The whole multi-scale modelling process chain is accelerated by automation and machine learning in every step, either by speeding up sample collection or by increasing the accessible length and time scales. Alternatively, machine learning is also applied when tackling the more difficult challenge of skipping the computational modelling entirely and predict metal hydride properties directly from compositions alone.

Copper- and Cobalt-based catalysts for photocatalytic hydrogen production

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Green hydrogen production, alongside reducing or capturing carbon emissions and recycling them, will be key components of a net-zero carbon future.¹ Hydrogen is already an industrially important chemical, and demand for green hydrogen is likely to increase, both in that role and in the energy sector (eg. reducing emissions from heavy transport) as we move to decarbonise in response to climate change.

Photocatalysis is one way of producing green hydrogen, through harvesting sunlight to provide the energy to drive suitable catalysts to split water into green hydrogen and oxygen. Studying model systems can help us find ways to improve such catalytic systems, for example looking at molecular cobalt² and copper³ catalysts under homogeneous photocatalytic conditions to help develop structure-activity relationships. Here we present our work on developing a robust homogeneous photocatalysis testing setup for hydrogen production here in New Zealand, along with preliminary results from testing some of our catalysts for hydrogen production under photocatalytic conditions in this new setup.

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Cyclic performance of iron ore-based oxygen carrier pellets using cement as the support during chemical looping biomass steam gasification for Hydrogen Production

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Biomass gasification is a thermochemical route to convert biomass into gaseous products mainly consisting of H₂, CO, CO₂ and CH₄. Adding steam as the gasification agent can promote H₂ generation through water-gas shift reaction, steam-char reaction and steam reforming of methane and tar.

Another factor for further enhancement is the selection of metal oxide-based oxygen carriers (OCs), which act as a lattice oxygen supplier and a catalyst for biomass steam gasification. In this way, H₂ yield increases and the OCs are transformed into reduced forms. With further gasification, reduced OCs catalyse the water-gas shift reaction and steam reforming of tars and methane. OCs can be reoxidised by air and then reused for the next cycle, and the cycling process is termed as chemical looping biomass steam gasification.

In this work, OC pellets developed by Hot Lime Labs, containing ironsand as active material and calcium aluminate cement as inert support, were applied in cyclic biomass steam gasification. XRD and SEM equipped with EDX spectroscopy were the main methods for OC characterisation.

The results showed that the cyclic performance of the OCs was affected by gasification temperature, attributed to the difference in the iron-based crystal phases. Shell exfoliation and occasional agglomeration were observed after 20 cycles of biomass steam gasification. It resulted in a gradual decrease in H₂ yield especially after 11 cycles. However, H₂ content in the product gas nearly remained at around 50%, the H₂/CO molar ratio was mostly above 2 and carbon conversion efficiency remained stable during the entire 20 cycles. Catalytic cracking of tars and methane also contributed to the H₂ production in this experiment.

Furthermore, the comparative investigation in this study indicated that both OCs and steam played a crucial role in boosting H₂ production, and steam helped to preserve the OC microstructure and retain its reactivity.

Demand response algorithms for industrial green hydrogen production

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Decarbonisation of industrial processes in New Zealand is a fast-developing space. Even hard to abate industries like steel are making significant changes to reduce carbon emissions. Green hydrogen production through water electrolysis provides a pathway to net-zero emissions for current hydrogen consuming industries (methanol, ammonia-urea and hydrogen peroxide). This work investigates the operation of a hydrogen production facility operating in a demand response regime. We propose a variety of algorithms to alter production in response to prices. Historical price data is used in the simulation and the impact upon production uptime and production efficiency are analysed.

Inflated and variable power prices are a significant barrier to industrial green hydrogen production. Flexible operating regimes like demand response are a simple method of reducing the price paid for power used. Electrolysis is a perfect technology to utilise this as it is easily able to alter electricity consumption in real time. This does not address the intermittency of renewable power but with increased electricity consumption renewable penetration increases which makes energy storage projects more viable. We found that a flexible operational regime decreased the cost per kg of hydrogen from ~4 NZD/kg to 0.06 NZD/kg when compared to an always on configuration. The demand response regime meant total production dropped by 82%, meaning a plant would need to be 5.6 times larger than the always on configuration. This leads to a classic CAPEX-OPEX trade-off where an algorithm can be used to achieve the desired electricity price.

Demand response operation of distributed green hydrogen electrolysis for industrial applications

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With New Zealand's push towards net zero greenhouse gas emissions by 2050, the industrial sector must undergo decarbonisation and look for sustainable alternatives for gaseous fuels. With New Zealand having a high percentage of the national grid supplied by renewable sources and continuing investment, green hydrogen produced via electrolysis is a potential solution. This work examines the feasibility of implementing grid-integrated electrolysis to produce hydrogen for the chosen case study of dairy processing plants in the greater Waikato region (that currently consume natural gas), with techno-economic and practical application considerations.

A challenge with grid integrated electrolysis is the intermittency of supply and the subsequent influence on the electricity market. Therefore, we propose the electrolyzers engage in demand response with historical data used for quantitative assessment. To mitigate price variability, distributed renewable generation is proposed for integration with the electrolyzers. Capital cost is typically high, which is addressed through electrolyzers distributed near power sources and existing gas infrastructure. The relative location to dairy processing plants is also considered. The proposed solution considers use of hydrogen fuel cells, as opposed to energy supplied by combustion of fossil fuels. Heat pumps are also considered in the implementation based on the overall energy requirements of the site. The sizing and geographical distribution of the solution's components are detailed, with an examination of how these may impact both expenditure (capital and operational) and greenhouse gas emissions. Impacts from policy and potential for sector coupling are also discussed.

Demand Scenarios for Hydrogen Transition in New Zealand: Priorities and Expectations

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Demand estimates are essential inputs for modelling the transition to a green energy system. We explored various hydrogen demand scenarios for New Zealand, building on current equivalent hydrogen amount for electricity, transportation, and industry feedstock demand levels, using Liebherr's famous Hydrogen Ladder to explore end-use cases.

We conducted a comprehensive analysis of hydrogen demand scenarios using a combination of qualitative and quantitative methods. Qualitative methods included interviews, written inquiries, and scenario planning exercises to identify key factors influencing hydrogen demand. Quantitative methods involved the use of conversion ratios, efficiency rates, and regional dissection of total hydrogen demand based on the density of feedstock supply to quantify the potential uptake of hydrogen across the transportation, industry, and energy sectors.

We clustered our results into three plausible hydrogen demand scenarios for New Zealand: a low case, a high case, and base case. The base case includes hydrogen use for fertiliser, methanol, and steel in the industry sector, in addition use for marine and aviation fuels in the transportation sector. Aviation and marine fuel demands incorporate large and medium-scale domestic and international voyages for commercial and passenger vessels. The low case incorporates the minimum demand for hydrogen, supporting the supply for methanol and fertiliser production only. For the high case, we considered all coastal and minor inland vessels in addition to the applications already mentioned in the base-case.

The role of hydrogen in New Zealand's energy future is uncertain, but it holds significant potential for reducing carbon emissions and contributing to a sustainable energy system. According to evaluated scenarios, we anticipate a hydrogen demand range of 0.24 to 1.17 million tons, with a base case assumption of 0.75 million tons for New Zealand. These scenarios will be used in energy transition planning for New Zealand.

Developing H₂ production catalysts by strategic installation of a synthetic cobalt core in protein scaffolds

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Catalytic H₂ evolution (HER) from water is considered a vital step in the pursuit of an H₂-mediated renewable energy infrastructure. The intrinsic instability of metalloenzymes under harsh practical conditions has led to the development of an array of synthetic H₂ production catalysts, which rarely match the exceptional performance of native enzymes. The omission of the critical protein scaffold enveloping the central metal active site is reckoned as the prime reason for this shortcoming.

This surrounding protein motif, known as the outer coordination sphere (OCS), remotely regulates the active site with synchronized electron and proton movement along with structural dynamics. Such an OCS feature has been replicated on the periphery of synthetic metal cores with multifunctional organic molecules that has significantly improved their native catalytic H₂ production.

This strategy was particularly successful with cobaloxime-based Co-N₄ cores that offer O₂-tolerant catalytic HER leading to the all-weather-ready catalytic assembly. However, the full potential of artificially designed OCS-decorated cobaloximes has not been realized due to the absence of an authentic protein scaffold.

Herein, we have deployed a series of rationally designed azurin (Az) protein scaffolds to explore their effect on promoting cobalt core-driven HER. Such an Az motif has been regularly utilized in several protein engineering studies and has a well-defined auxiliary coordination sphere. The successful construction of the cobaloxime-Az dyad resulted in a significantly enhanced electrocatalytic HER in aerated water, highlighting the prospects of this bio-inspired catalyst design approach.

Development of a Lab-Scale Plant for Renewable Energy and Hydrogen Research

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Broad availability and decreasing cost of both renewable energy generation and hydrogen technologies is enabling a transition away from fossil fuel-based energy. Combined, these approaches enable the generation of green hydrogen; a carbon-free energy carrier that can facilitate scalable storage and distribution of renewable power.

However, assembling infrastructure for optimal production of green hydrogen is challenging, as a broad spectrum of technologies from the domains of power and electronics engineering, electrochemistry, internet of things (IoT), and software must be integrated into cohesive plant architectures. Moreover, the energy sources tapped by such plants – namely wind and solar – are ephemeral in nature and difficult to predict accurately. Industry 4.0 paradigms promise to optimise operation of hydrogen plants through greater connectivity, intelligent decision making, and advanced analytics to achieve peak hydrogen production from limited or inconsistent energy input. Experimentation and development within this space is challenging, as even at a pilot-scale plant equipment must conform to various hazardous area codes.

This work presents progress on development of a lab-scale hydrogen plant test-bench designed for experimentation and benchmarking of renewable, hydrogen, and industry 4.0 technologies. The plant integrates lab-scale solutions for photovoltaic (PV) emulation, a micro-grid with battery storage, hydrogen electrolysers and fuel cells, and gas storage, all backed by calibrated electrical instrumentation for metric collection.

The plant is designed to allow individual components be swapped out for custom or commercial equipment to study performance as part of a facsimile of a real-world plant, and to facilitate experiments with software models such as digital twins. The plant is operated by custom modular software that facilitates data collection and aggregation, and utilises cloud services for data analysis and visualisation. Hardware designs and software will be released under open-source licences, providing reference for industry and academia to establish their own test-benches.

Development of Photoanodes and Proof-of-Concept Photoelectrochemical Cell for Green Hydrogen Production

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Global greenhouse gas emissions have increased significantly since the beginning of the industrial revolution in the late 18th century. These human-driven emissions have been the result of an increase in demand in the energy, industrial, transport, and land use sectors.

Photoelectrochemical (PEC) water-splitting, often referred to as artificial photosynthesis is considered by some as a “holy grail” of renewable energy, producing hydrogen fuel directly from solar energy.

Bismuth vanadate (BiVO_4) has shown promise as a photoanode material for both PEC water-splitting, absorbing a significant range of the solar spectrum and having favorable band edge positions. However, the material suffers from poor electron-hole pair recombination, reducing its performance. The cause of recombination is largely underreported in the literature.

In this study, Intensity-modulated photocurrent spectroscopy (IMPS), an electrochemical technique able to deconvolute bulk and surface properties of a photoanode material was used to develop a high-performing photoanode material consisting of an optimized Molybdenum-doped BiVO_4 photoanode with an Fe/NiOOH cocatalyst layer. Reducing recombination in the material, the optimized photoanode could reach photocurrent densities greater than 1 mA/cm^2 at 1.23 V vs. RHE. Physio-chemical techniques such as scanning electron microscopy (SEM) and x-ray diffraction (XRD) were used to characterize the material and a range of electrochemical techniques were also used to measure the performance of the material.

For the first time, IMPS was also used in operando during stability testing to identify areas of degradation in the photoanode material. The stability weaknesses discovered in this study can be targeted to increase the longevity of the material. A proof-of-concept cell utilizing the photoanode material was also developed. The cell with an 80 cm^2 active area was used to determine the solar-to-hydrogen efficiency of the material.

Direct reduction of New Zealand sands to hydrogen storage material

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Iron-titanium-based alloys are promising materials for large-scale hydrogen storage applications. New Zealand has a large deposit of raw materials containing iron and titanium in the form of oxides; among them is ilmenite (FeTiO_3). Potentially, this material, once reduced, might be a cheap and abundant source of hydrogen absorbing TiFe alloys.

This poster shows the challenges and first results on reducing ilmenite with the help of hydrogen, calcium, magnesium or a mix of these elements. Two reduction methods are presented, the first of which involves the mechanochemical reduction of ilmenite via ball milling and the second involving the treatment of ilmenite at high temperatures. The thermal reduction treatment is analysed in detail with synchrotron data and differential thermal analysis (including mass spectroscopy). This research is in the framework of the German-New Zealand Green Hydrogen Centre 'He Honoka Hauwai'.

Driving the transformation to hydrogen ironmaking: An experimental vertical shaft H₂-DRI reactor facility at Robinson Research Institute

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Iron and steel production account for approximately 6.3% of global anthropogenic CO₂ emissions. Direct reduction of iron with hydrogen emerges as a promising approach for decarbonizing the iron and steel industry. Extensive small-scale laboratory experiments have assessed the viability of hydrogen-direct reduction of iron ores from diverse geographical sources.

However, these batch laboratory results don't necessarily translate to continuous commercial-scale processes. The establishment of a small-scale continuous test reactor for the H₂-DRI process is challenging, demanding significant resources and investment. The scarcity of small-scale reactors suitable for testing under relevant conditions presents a major hurdle in the development of H₂-DRI, creating a substantial gap between laboratory success and proof of commercial feasibility.

This presentation outlines the recent commissioning of a continuous counter-flow vertical shaft reactor, boasting a processing capacity of 6 kg/hr for iron ore pellets with an H₂ flow of up to 100 NL/min. Notably, this reactor stands as the largest H₂-DRI facility in the Southern Hemisphere. In this talk, we will discuss the design and construction journey for this reactor, spanning from the initial system design to the successful demonstration of H₂ reduction on titanomagnetite ironsand pellets.

This reactor now enables a range of research capacities, including the validation of laboratory findings on a larger scale with practical operational variables. It allows for the assessment of the feasibility of hydrogen direct reduction for different iron ores on a commercial scale, identification of scalability issues, adherence to operational parameters, and mitigation of potential challenges before the construction of a full-scale plant.

Moreover, it provides a practical solution for producing small-quantity DRIs for downstream melting investigations. In essence, this newly commissioned research facility presents significant benefits in advancing the transformation of iron and steel production toward a more sustainable and environmentally friendly industry.

Effect of Ilmenite reduction pathway on TiFe hydrogen storage properties obtained by Sieverts apparatus measurement

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On the west coast of New Zealand, large amounts of natural ilmenite (TiFeO_3) ore in the form of black sand can be found. This easily accessible oxide might be reduced to a titanium-iron alloy by different pathways. The simplest approaches use reducing agents at high temperatures. After purification, the obtained alloy has the potential to become an abundant and cheap material for large-scale hydrogen storage applications. In this work, we investigate the effects of the reduction process on the hydrogen storage capacity, thermodynamics, and kinetics of the synthesized TiFe alloys.

The ilmenite purified from New Zealand ore was reduced at Victoria University of Wellington under various experimental conditions, e.g., temperatures, durations, and grind sizes. The TiFe samples were thermally activated under dynamic vacuum after some hydrogen adsorption and desorption cycles were measured. The hydrogen uptake properties of the alloys can be determined using a specially built Sieverts apparatus. The gravimetric storage and kinetics of the samples will be evaluated by numerical fitting to remove errors from the apparatus.

Effect of Mechanical Alloying on Phase Synthesis and Hydrogen Absorption/ Desorption Behavior of (TiV)₅₀(CrMnFe)₅₀ Alloys

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Efficient energy storage is paramount to address global energy demands and environmental concerns. Hydrogen, as a clean and high-energy-density fuel, holds great promise. However, conventional hydrogen storage methods encounter limitations in safety, density, and transportation. Hydrogen storage alloys, by adsorbing hydrogen within crystalline structures, present an efficient storage solution.

This study investigates the impact of mechanical alloying processes on the phase synthesis of (TiV)₅₀(CrMnFe)₅₀ hydrogen storage alloys by systematically varying milling time, ball-to-powder ratios, and milling speeds. Complementary characterization techniques, including X-ray diffraction (XRD) and scanning electron microscopy (SEM) equipped with energy-dispersive X-ray spectroscopy (EDS), are employed to analyze the resultant alloy's phase constitutions and microstructures. High- pressure differential scanning calorimetry (HP-DSC) is utilized to examine the initial hydrogen absorption/desorption behavior of the alloys.

The results indicate that, at a ball-to-powder ratio of 10:1, a milling speed of 350 rpm, and a milling duration of 15 hours, the material underwent successful alloying, and closely approximating its designed composition. The material is primarily composed of the BCC solid solution phase, with minor constituents of the Laves phase. These findings underscore the capability of mechanical alloying to prepare materials with the desired phase constitutions, with virtually no segregation compared to traditional melting process. Subsequently, high-pressure DSC results suggested that the alloy's initial hydrogen absorption/desorption occurred at relatively low temperatures before activation. Hydrogen absorption was noted around 120°C, and hydrogen desorption occurred around 200 °C.

Effects of catalysts on the capacities of HPSB hydrogen storage material

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HPSB hydrogen storage material is a kind of porous lamellar structural material developed by our research group. Due to the special structure of this material, it can absorb hydrogen at room temperature, hydrogen absorption pressure is 2-4MPa, and hydrogen absorption time is 2-5min.

The main preparation method used in the experiment is hydrolysis. The main raw material is sodium borohydride, and the reaction temperature is 30°C.

In this experiment, in order to improve the hydrogen storage performance of HPSB hydrogen storage material, Co-B and samarium oxide were introduced as catalysts during the preparation of HPSB.

The results show that the amount of samarium oxide and the ratio of samarium oxide to Co-B have obvious influence on the hydrogen storage performance of HPSB. In addition, according to the results of SEM analysis, the amount of samarium oxide and the ratio of samarium oxide to Co-B also have obvious effects on the microstructure of HPSB hydrogen storage materials.

Effects of ion irradiation on molybdenum disulfide films for hydrogen evolution reaction

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Electrocatalytic water splitting using renewable energy for green hydrogen (H₂) production is an attractive strategy to reduce CO₂ footprint [1]. Developing efficient and cost-effective catalytic materials has been at the forefront of green H₂ research activities [1,2]. Ion beam engineering is a promising method to improve electrocatalytic performance for enhanced hydrogen evolution reaction (HER) [3]. This is achieved by controlling ion beam irradiation parameters such as ion species, ion beam energy, and fluence (ions.cm⁻²). Molybdenum disulfide (MoS₂) is a technologically important semiconductor with interesting catalytic activities [4,5].

Here, we report the HER results of Ni implanted MoS₂ thin films. The MoS₂ films were fabricated by ion beam sputtering method [6]. Rutherford backscattering spectrometry results showed films to be sulfur deficient (MoS_{2-δ}). Hexagonal 2H MoS₂ phase was confirmed with X-ray diffraction. The MoS₂ were implanted with Ni between 5×10¹⁴ and 5×10¹⁵ ions.cm⁻² which yields around 0.5–4.5 at% Ni located at ~15 nm below the surface. Contact angle measurement results showed that the contact angle values decreased with increase in Ni fluence suggesting more hydrophilic films. Electrochemistry measurements showed that the film implanted with 1×10¹⁵ Ni.cm⁻² exhibited an enhanced current density with a lower onset potential of 510 mV compared to 545 mV for un-implanted film. Detailed results from compositional, structural, morphological, and electrochemistry measurements supported with ion beam simulations will be presented in the symposium.

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Efficient LDH materials for OER catalyst in direct seawater splitting

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Water splitting has been identified as a promising future technology to produce clean hydrogen. However, most existing research uses fresh water or processed seawater, which either consumes freshwater resources or entails additional energy and financial costs to process seawater. Thus, direct seawater splitting is essential to preserve freshwater resources for human consumption and irrigation, and reduce expenses associated with future hydrogen industries.

A significant challenge associated with direct seawater splitting is the occurrence of the Chlorine Evolution Reaction (CIER) at the anodic side, which can seriously interfere and compete with the Oxygen Evolution Reaction (OER), resulting in the production of chlorine/hypochlorite. This chemical reaction can cause damage to equipment or hardware as well as pollute the environment.

In this work, our newly developed NiFeMn LDH catalyst exhibits superior selectivity on OER over CIER with high electrochemical activity. The doping of Mn demonstrated a great effect on the OER selectivity and performance improvement.

Electro-catalytic CO₂RR by immobilizing molecular complexes onto a carbon support

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The conversion of energy-poor feedstocks such as water or CO₂ into energy rich molecules like H₂ or methane, methanol, etc., or higher carbon products, driven by renewable energy, has emerged as a promising pathway for producing future eco-fuels and industrial chemicals. As these conversions are energy intensive, catalysts are required to reduce the energy required to convert such feedstocks, and to provide selectivity with regard to the product obtained.

Molecular complexes for CO₂ reduction are of interest as they provide the potential to develop structure activity relationships, which in turn enable predictable activity tuning by modifying the ligands or by incorporating different transition metal ions such as Cu, Ni, Co or Fe, with the aim of providing selectivity for a particular higher carbon product.¹ Although many molecular complexes have shown promising activity towards CO₂RR, the commercial viability of these complexes is limited by instability, limiting catalysis lifetimes. However, enhanced stability can be achieved by immobilizing these molecular complexes onto various carbon supports, such as carbon black, reduced graphene oxide or carbon nanotubes.² This project is focused on the immobilization of mixed metal complexes onto a carbon support for electro-catalytic CO₂RR.³ Results from these studies will be presented.

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Electrochemical Ammonia Production Based on Transition Metal Nitrides

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Ammonia (NH₃) is the world's second-most-produced chemical, accounting for 2% of global energy supply and carbon emissions each year. The electrocatalytic nitrogen reduction reaction (ENRR) poses as one of the environmentally friendly alternatives for decarbonising and ensuring sustainable production of NH₃. Among ENRR electrocatalysts, transition metal nitrides (TMNs) have a potential advantage for continuously making NH₃ through its unique mechanism, known as the Mars-van Krevelen (MvK) pathway.

For this conference, we present our recent progress on the development of TMNs electrocatalysts via nitrogen ion implantation on transition metal thin film, then using them as working electrodes in our custom-built electrochemical reactor. Comprehensive characterisation were conducted to examine the elemental compositions and structural properties. The electrocatalysts performance of the N- implanted electrocatalysts were compared under an argon and nitrogen saturation at ambient conditions. Outstanding catalysts were further tested to validate the formation of ammonia via Mars van Krevelen mechanism. Overall, this research is expected to shed light on the challenges of designing ENRR electrocatalysts with respect to high selectivity towards ammonia production, as well as with chosen strategy for overcoming practical difficulties in this field.

Electrochemical conversion of nitrate to green ammonia as an alternative hydrogen carrier

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Ammonia (NH₃), a crucial component in fertilizer production and a potential green fuel, has attracted increasing attention due to its role in sustainable energy and H₂ carrier applications. Traditional ammonia production processes, however, are energy-intensive and emit massive CO₂. The paradigm transition towards green ammonia production involves exploring environmentally friendly synthesis methods.

This study addresses the challenge through the electrochemical reduction of nitrate to ammonia, presenting a dual-atom catalyst approach with CuFe-based materials. As the demand for sustainable energy storage solutions rises, the role of ammonia as a high-capacity hydrogen carrier gains prominence. Our research contributes to this landscape by developing efficient, selective, and stable catalysts that facilitate the electrochemical conversion of nitrate to ammonia.

The CuFe dual-atom catalysts, designed and optimized for enhanced electrocatalytic performance, exhibit outstanding efficiency in promoting the nitrate reduction process (over 300 mmol/h/g of ammonia yield rate with a faradaic efficiency of 99% at -0.62 V vs. RHE). Through full characterization, theoretical calculation, and systematic analysis, we unravel the synergistic effects of dual-atom configurations, shedding light on the intricate catalytic mechanisms at play.

This work not only establishes a novel avenue for the electroreduction of nitrate to produce ammonia but also aligns with the broader objectives of sustainable ammonia synthesis. The implications of our findings extend to the realm of H₂ carrier and storage systems, presenting a potential breakthrough in environmentally friendly energy conversion technologies.

In conclusion, the utilization of CuFe dual-atom catalysts presents a promising step towards sustainable and efficient ammonia synthesis, contributing to the evolving landscape of green ammonia production and its applications in H₂ carrier and storage systems.

Electrochemical Reduction of Carbon Dioxide

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Sustainable technologies focused on carbon dioxide utilisation are essential if we are to shift to new sources of energy supply and mitigate climate change. Among the technologies developed so far, those based on electrochemistry, which utilize electricity from intermittent renewable sources as the energy input, are particularly attractive since they offer excellent scalability for industrial implementation. Commercially feasible electrochemical processes for carbon dioxide utilisation require the use of highly stable, selective and active catalysts to overcome high energy barriers associated with the relevant reactions. In recent years, nanoengineering strategies have been applied to develop more advanced electrocatalysts [1,2]. With the assistance of advanced instrumental characterization tools and more sophisticated density functional theory calculations, significant progress has been made in the development of advanced electrocatalysts [3,4]. To fully realize the potential of electrochemical CO₂ reduction technology for commercial application, more advanced gas diffusion electrodes have been developed [5,6]. This talk highlights the recent progress in the electrode/electrocatalyst design and mechanistic study made by the Monash Electrochemistry Group.

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Electrochemical testing in gas diffusion electrode (GDE) half-cells: Bridging the gap between model thin film and realistic fuel cell operation conditions

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Proton exchange membrane fuel cells (PEMFCs) are highly efficient energy conversion devices, and Pt catalysts are considered optimal for industrial standards in PEMFC devices. However, since Pt is both expensive and non-sustainable, much scientific effort has been devoted to finding efficient, durable and low-cost electrocatalysts. These new electrocatalysts require solid benchmarks to evaluate oxygen reduction reaction (ORR) activity for example, and performance in a laboratory scale model should match their eventual performance in realistic devices.

Rotating disc electrodes (RDE) are routinely used for testing, but they fail to mimic real fuel cell conditions in terms of water management, ionomer distribution and relevant current densities. In addition, the mass transport between the thin catalyst layer (CL) in RDE experiments and the CL on a gas diffusion layer, as used in industrial Membrane-Electrode-Assemblies (MEA), differs a lot. MEA experiments can therefore help to evaluate the contribution of CL effects to performance, but they are time and cost inefficient and cannot provide insight into the individual electrode processes.

To combine the benefits of both techniques, electrochemical half-cell set-ups with gas diffusion electrodes (GDE) are used to characterize novel electrocatalysts. They can imitate the three-phase boundary and ionomer distribution of MEAs, while being fast and reproducible under standardized test conditions. Realistic operational conditions, such as potential range and higher current densities in the GDE setups, are more similar to MEA testing than RDE, without the hassle and cost of full-cell tests.

But several parameters need to be considered when performing GDE half-cell tests, such as the cell design and measurement variations. Therefore, this presentation will discuss the effects of different flow fields to control the gas flow through the cell as well as the importance of the ohmic drop compensation (iR) and different methods for its implementation like Staircase Galvano Electrochemical Impedance Spectroscopy method.

Engineering defects in TiO₂ for the simultaneous production of hydrogen and organic products

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Photoreforming ethanol to simultaneously produce hydrogen and value-added organic products was realized over defective TiO₂. Chemically induced defects in TiO₂ promoted light absorption and charge separation, enhancing overall photoactivity.

The induced defects also regulated product selectivity, leading to greater hydrogen purity and liquid-to-gaseous carbon ratio. The optimal catalyst generated 0.08 mmol/hr of hydrogen with a purity greater than 99 % and 0.08 mmol/hr of liquid acetaldehyde over a 6 hr timeframe. This was three times greater than the untreated TiO₂. Active species trapping revealed that the preferred ethanol oxidation pathway was direct hole transfer, indicating that selectivity relies on surface chemisorption. Surface defects decreased the acetaldehyde adsorption energy, instigating its prompt desorption and suppressing overoxidation into CO₂, thus improving the selectivity towards hydrogen and liquid hydrocarbon products.

The work offers an alternative approach towards sustainable energy by coupling photocatalysis with waste organic utilization.

Enhanced photocatalytic H₂ production by matching blue edge with absorption edge in TaON photonic crystals

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In this study, tantalum oxynitride inverse opal (TaON IO) photonic crystals with different macropore diameters (D) were synthesized in a two-step process involving colloidal crystal templating and thermal nitridation, then applied as visible light-driven photocatalysts for hydrogen production.

The TaON IOs showed photonic band gaps (PBGs) at visible wavelengths, with the PBG position redshifting as the diameter of the macropores increased in accordance with a modified Bragg's law expression. By aligning the electronic absorption edge of TaON ($E_g \sim 2.4$ eV) with the blue edge (short-wavelength side) or red edge (long-wavelength side) of the PBGs, slow photon enhancement of photocatalytic H₂ generation was realized. H₂ production tests conducted in 10 vol% methanol containing H₂PtCl₆ under Xe lamp irradiation (150 W) showed that the hydrogen production rate was enhanced by ~ 1.3 – 1.4 times when the TaON absorption edge (~ 510 nm) aligned with blue edge of the PBG (0.3421 mmol g⁻¹ h⁻¹) or the red edge of the PBG (0.3254 mmol g⁻¹ h⁻¹) in the inverse opals. The red edge enhancement was due to increased light absorption and charge carrier generation in TaON, whereas the blue edge effect was likely due to suppression of electron-hole pair recombination.

Results demonstrate that photonic crystal engineering to exploit slow photon effects is a viable approach for boosting photocatalytic hydrogen production rates.

Enhancing Electrocatalysis via Mechanical Energy Conversion

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Catalytically driven Hydrogen production will revolutionise the energy industry.

Here, I will discuss our approach to lowering the required electricity input for hydrogen production - by exploiting motion & mechanically responsive materials.[1] The kinetic effects, such as improved mass diffusion, achieved through vibration are coupled with electronic effects, such as band screening and fermi level shifts from the mechanically responsive materials.[2]

Our approach is enabled by self-poled polymer piezoelectric materials.[3] To lower the energy input, these fluoropolymers are directly coupled to water splitting electrocatalysts. By controlling the interface between the electrocatalysts and the polymer and applying random or repetitive motion, the electronic structure of the catalysts is locally altered. Dependant on the polarisation vector of the polymer,[4] this allows the catalyst to function at either more positive or more negative applied potentials. The piezo-electrocatalysts can generate an improvement in current of over 33% compared to electrocatalysis at static overpotentials. Whilst achieving identical current densities at 500 mV lower overpotentials.

The fundamental principles discussed can be applied broadly to portable and scalable future fuel production, providing a pathway to low energy fuel production.

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Exploring energy futures through green hydrogen's sociotechnical narrative

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As a flexible vector, hydrogen presents an opportunity to replace fossil fuels and to decarbonise some 'hard to electrify' sectors such as heavy transport, aviation, steel and fertiliser production. The narrative of green hydrogen presents a satisfying technological fix to many difficult transition issues. But this suggested 'smooth transition' appears to generate concern as well as optimism.

Based on interviews with selected experts across New Zealand, this research suggests that the dominant ways that green hydrogen is discussed may actually limit our capacity for imagining more creative and just energy transition solutions.

Critiques of the dominant green hydrogen narrative show that this technology's 'business as usual' approach has the potential to perpetuate contemporary energy system issues, suggesting that replacing fossil fuels is not enough to encourage social transformation.

However, these critiques also suggest that there are opportunities to reimagine green hydrogen applications that better align with notions of energy justice and democracy.

Exploring Green Hydrogen's Place in the Green Future of Aotearoa, New Zealand – Perspectives from Southland

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In accordance with the 2015 Paris Agreement, Aotearoa, New Zealand aims to reach net zero carbon by 2050 - this has posited unique opportunities and challenges for industries to decarbonise. Green hydrogen is one solution to decarbonise some of Aotearoa, New Zealand's energy sector.

In recent years, the green hydrogen industry has seen massive interest as it promises to decarbonise 'hard to abate sectors' such as heavy transport. Green hydrogen is a technology that requires input, dialogue and development by many stakeholders to become part of a viable solution to Aotearoa, New Zealand's growing need for green energy.

Because of this, this paper approaches the development of green hydrogen within Aotearoa, New Zealand through a broad approach. Using a multidisciplinary (sustainable business, social science, and natural science) lens, stakeholder interviews were analysed through both multi-level perspectives and energy cultures.

This paper presents an opportunity for deeper research into the industry of green hydrogen and how this new technology will contribute to the green futures pathway specifically in the Southland region.

Fast power regulation method of electrolytic hydrogen production load based on silicon controlled rectifier with power electronic on-load-tap-changing switches

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The electrolytic hydrogen production (EHP) based on renewable energy is a promising hydrogen production method, whereas due to the fluctuation of renewable energy, the EHP load should possess fast power regulation capability to maintain power balance. In this paper, a fast power regulation method of silicon controlled rectifier (SCR) with power electronic on-load-tap-changing (OLTC) switches is proposed, and it can overcome the drawback of slow response of existing SCR with mechanical on-load-tap-changing switches, which is suitable for large scale electrolyzer. The simulation results are provided to verify the effectiveness of proposed method.

Future hydrogen infrastructures – a European perspective

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The transformation of the energy system requires extensive adjustments to the infrastructure. Due to the geographically different and temporally variable availability of renewable energy sources such as wind, solar and hydro power, future grid infrastructures and temporal balancing through storage and demand flexibility are crucial.

This contribution focuses on flexible sector coupling, transport networks and their interaction in the future energy system of Europe. It presents the current state of planning for the deployment of hydrogen infrastructures.

In addition, it summarizes the results from various energy system studies that deal with the role of hydrogen in Europe's future energy system. The modelling results show the potentials of a conversion of gas grids to hydrogen, but also the high dependency of the infrastructure design on political decisions.

This particularly concerns the development of the demand for hydrogen, the preferred power sources as well as the ambition for a high self-supply share.

Grain refinement of Mg-RE based hydrogen storage alloys prepared by amorphous-crystallization technology

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Mg based hydrogen storage alloys with nanocrystalline microstructure were prepared by the amorphous-nanocrystallization route. Grain refinement and stabilization of the nanocrystallized alloys were improved by enhancement of the nucleation rate and introduction of the secondary phase pinning effect. The nucleation characteristics which were directly related to the crystallization kinetics can be tailored by the chemical composition and crystallization processes.

The secondary phase pinning effect can be dramatically strengthened by the low-energy interface configuration between the phase structures. The mechanisms were discussed from the point views of thermodynamic, crystallization kinetic and crystallographic considerations. The fine nanocrystalline favored the hydrogen storage kinetic properties.

Green hydrogen production potential at city level: A GIS-based approach for New Zealand

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Green hydrogen and its derivatives have gained momentum as versatile energy carrier to support the energy transition, yet their implementation need to be understood. Increasing cost and technological complexity of transport and storage of hydrogen underscore the importance of designing green hydrogen production sites in proximity to their ultimate end-use destinations.

Here, the geospatial context plays a large role, specifically understanding how to integrate hydrogen applications, from the production to transportation to the end-user into existing urban infrastructure.

Our study highlights New Zealand's untapped renewable energy generation and hydrogen production potential, beginning with solar. We use FlexiGIS-H₂, a GIS-based optimisation model, to derive a city's urban energy infrastructure, categorising buildings of different sectors based on land-use and deriving their electricity demand based on corresponding demand profiles.

Open-source geographical data is used to calculate electricity generation potential from available rooftop areas and surplus energy is allocated to hydrogen production. We then strategically site green hydrogen production facilities in proximity to end-users. Insights into local green hydrogen production prospects will be exemplified by a comparative analysis between Christchurch and Auckland. The resulting potentials, load and generation curves, as well as production sites are relevant to local planners and can also be used for national pathway planning.

Highly sensitive and selective hydrogen gas sensors employing photoactive hybrid nanomaterials

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Hydrogen - an odorless and colourless gas - is highly flammable (ignition energy: 19 μ J) and explosive (4-75%) [1-4]. Development of accurate, reliable, and selective hydrogen gas sensors is crucial for industrial activities that utilize hydrogen as a clean energy carrier while maintaining safety. A new class of hydrogen sensors based on photoactive hybrid nanomaterials are now emerging with enhanced sensing performance (low-operating temperature, high sensitivity and selectivity, low limit of detection, and long-term stability) [2-4]. Under illumination from an appropriate light source, photogenerated electrons and holes are formed in the conduction and valence bands leading to an increase in the carrier density and the number of active sites, enhancing sensing performance.

TiO₂ nanomaterials - photoactive semiconductive metal oxide - are promising candidate for hydrogen sensing due to their large surface-to-volume ratio, increased active sites, and tuneable bandgap properties allowing them to function effectively under light conditions. In this research, we have developed hybrid materials comprising of TiO₂ nanospheres (NS), Pd nanoparticles, and reduced graphene oxide (rGO) (e.g., Pd/TiO₂, Pd-PdO/TiO₂ and rGO-Pd/TiO₂). SiO₂ nanospheres have also been used as a template to make the TiO₂ nanospheres hollow. The synthesised materials have shown promising results towards hydrogen at low operating temperatures (e.g., 25-35°C) with high sensitivity and selectivity and fast response and recovery (14s/53s). In this talk, material synthesis and characterisations as well as hydrogen gas sensing results and mechanisms will be discussed.

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Hydrogen Evolution on a Pt Single Atom

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Single-atom catalysts (SACs) have been gaining attention in electrochemical catalysis for their high atom-utilization efficiency, minimizing the need for bulk precious metals such as Pt. However, typical measurements average the electrochemical signals from many single atoms that are dispersed across a large electrode. This makes it impossible to isolate the electrochemical response from each individual SAC.

Scanning electrochemical cell microscopy (SECCM) uses a pipette that is hundreds of nanometres in diameter to isolate small areas of an electrode surface for electrochemical measurements. Using a SECCM approach, we demonstrate that it is possible to isolate the electrocatalytic hydrogen evolution reaction on a single Pt atom.

Hydrogen Generation and Storage: from Materials to Components

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Hydrogen technology will play an important role in our future sustainable energy economy as well as for zero-emission mobility. Hydrogen will also open opportunities for global energy partnerships and can thus facilitate energy autonomy and political resilience.

Recent research on materials for efficient renewable generation and reversible storage of hydrogen will be presented. Different aspects from basic materials development to systematic science-based scale-up and system design will be covered, including in-operando experiments as well as modelling and simulation.

Green hydrogen can be efficiently generated by solar water splitting in photo-electro-chemical cells. Respective photoactive TiO_2 , BiVO_4 , Fe_2O_3 , or WO_3 coatings are produced by kinetic (aerosol) spraying, and show high photo-currents.

Solid nanostructured hydrides offer a safe, compact, and energy efficient hydrogen storage solution for stationary as well as mobile applications. Highest energy efficiencies can be achieved, if operation temperature and reaction enthalpy are tailored for the particular system integration, e.g. with a fuel cell. Current projects geared towards hydrogen integration in stationary and mobile applications will be presented.

Hydrogen Generation from Cyclic and Acyclic Carriers using 3D Catalyst Technology

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¹CSIRO

Carriers containing chemically stored hydrogen offer an excellent pathway to bind hydrogen for safer storage and transportation, and for clean fuel generation.

Therefore, hydrogen carriers such as ammonia and LOHCs are receiving significant interest in development of alternate technologies for optimal hydrogen storage and generation. CSIRO has developed a new structured catalyst platform that can be used for hydrogen generation from these carriers in a robust and efficient manner.

These 3D-printed catalytic scaffolds or Catalytic Static Mixers (CSMs) offer several advantages over conventional catalyst packed bed systems (PBS) in that they offer negligible pressure drop, predictable and tuneable flow field, and the metallic scaffold offers efficient heating and improved catalyst performance.

Thus, these CSMs act as great technological alternative to conventional catalyst systems for hydrogen reforming at high temperature/pressure. A novel 3D scaffold, coated with the catalyst of choice, is used for the thermochemical dehydrogenation of the substrate (aka H₂ carrier).

The experiments are performed inside a tubular flow reactor, under high temperature/pressure conditions. Sample analysis is performed using NMR or gas chromatography to identify process efficiencies.

This work will involve catalyst screening and investigating the influence of process parameters on reaction kinetics. Initial experiments show promising conversions in the system using CSMs (~55% for LOHCs and >99% for ammonia) which shows the potential of the CSM technology in hydrogen generation. Through further design and process optimization, it can serve as a robust alternative to conventional catalyst systems.

Hydrogen Migration Within Earth

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Understanding the mechanisms of large-scale, subsurface hydrogen migration is essential for natural hydrogen exploration and for hydrogen storage assessment. The unique properties of hydrogen make that the timescales of hydrogen migration through the deep and shallow

Earth and within geological basins vary from billions to thousands of years. Within the deep Earth, advection of hydrogen-enriched rocks from the lower mantle delivers material to a variety of geological settings, including Mid Ocean Ridges and hotspots.

Within the shallow Earth, diffusive and advective transport mechanisms are dependent on a wide range of parameters including geological structure, microbial activity, and subsurface environmental factors, e.g., salinity, temperature, and pressure. Furthermore, the provenance of sedimentary rocks that contain material from Archean - Proterozoic crystalline basement rocks are also an important factor in subsurface and fluvial hydrogen migration.

In this study, we extensively review the nature and timescale of hydrogen migration from the planetary to basin-scale, and within both the deep and shallow Earth. We explore the role of planetary accretion in setting the hydrogen budget of the lower mantle, propose a conceptual framework for primordial hydrogen migration to the Earth's surface and evaluate its role in setting the hydrogen budget of the rocks delivered from the deep Earth. We also review the mechanisms and timescales of hydrogen within diffusive and advective, fossil and generative and within biologically moderated systems within the shallow Earth. Finally, we assess the challenges of and discuss potential methods for modelling basin-scale hydrogen migration.

Hydrogen reduction of raw and pre-oxidised NZ titanomagnetite ironsands in a small-scale high-temperature fluidised bed

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The use of hydrogen as a reducing agent can substantially reduce CO₂ emissions from the ironmaking process. Iron ore fines can be reduced in a fluidised bed using hydrogen at high temperatures (>800°C), although several studies have reported sticking of particles which causes the bed to defluidise, effectively shutting down the process.

Here, we report results from the reduction of NZ titanomagnetite ironsands in a small-scale laboratory fluidised bed (100 g) at temperatures between 800-1000°C using H₂ flow rates up to 5 SLPM. No sticking phenomena are observed under any of these conditions, which is attributed to the formation of a stable titanium-bearing oxide layer on the exterior of each particle, that prevents iron-iron contact at the particle surfaces. Pre-oxidised NZ titanomagnetite ironsands have also been studied and shown not to stick. Interestingly, at lower reaction temperatures the reduction kinetics for pre-oxidised ironsands is faster than for raw ironsands.

This increased kinetic rate can be attributed to the pre-oxidation stage inducing micro-fractures that create a void for the hydrogen to diffuse into the inner regions of the particle. The findings are important as increasing the operating temperature of the fluidised bed reactor results in a faster reaction rate and higher gas utilisation, making the process more economically attractive.

Hydrogen storage materials: Challenges and opportunities

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Materials-based hydrogen storage via chemical bond has attracted strong interest. Chemical hydrogen carriers featuring B–H, C–H, N–H, and O–H bonds have been studied extensively, such as methanol, cyclohexane, and ammonia. Due to the low costs, widespread infrastructure, and solid understanding of their chemical properties, these compounds are being seriously tested as hydrogen carriers.

However, these compounds also have some disadvantages such as high temperatures required for (de)hydrogenation, slow kinetics, high energy required for regeneration. For practical applications, a holistic understanding of these particular types of hydrogen carriers is needed. This talk will present an overview of these compounds featuring B–H, C–H, N–H, and O–H bonds, and discuss strategies employed to improve the hydrogen cycling performance.

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Initial investigation into the in-flight reduction of New Zealand ironsand.

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The current method for the reduction of iron sand to metallic iron in the steel making process relies on carbon as the primary reducing agent. The ability to reduce ironsand using hydrogen would remove the need for carbon in this process, and hence decrease the carbon footprint of this process.

Here, we report an initial experimental investigation into the pre-reduction of New Zealand ironsand during high temperature argon-hydrogen plasma spraying. New Zealand ironsands were fed into a plasma gun and sprayed onto a bronze substrate under an argon-hydrogen gas mixture at various feed rates to probe the effect of changing the powder to reductant gas ratio.

Despite powder residence times in the plasma spray of ~100ms, we found that the first stage of reduction to wustite (FeO) was largely completed, and that the feed rate of the powder did not make a significant difference across the experimentally studied range. Our results show that hydrogen plasma-spray reduction offers promise as a novel approach towards realising towards direct 'zero-carbon' steel smelting.

Interface Controlled Nanocatalysis for Hydrogen Evolution

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Hydrogen has emerged as a green and sustainable fuel to meet the demand for future global energy. Nowadays the majority of hydrogen is still produced from steam-reformed methane, which is derived from limited fossil resources and greatly increases CO₂ emission.

Electrocatalytic hydrogen evolution reaction (HER) enabled by renewable electricity holds great promise as a safe, scalable, low-cost, and environmental-friendly pathway for hydrogen production. To date, noble metals (e.g., Pt, Pd, and Rh) are regarded as the most efficient materials to catalyze the conversion of H₃O⁺ (acid) and H₂O (alkaline) to H₂. In order to maximize the utilization efficiency of noble metals, the rational design and controllable synthesis of catalysts based on the deep understanding of reaction mechanism and structure–activity relationship is crucial for cost-efficient HER catalytic process.

In this talk, I will summarize and discuss our recent work for the development of interface controlled nanocatalysis for HER, including the fine control over the oxidation states of single-atom Pt catalysts through electronic metal–support interaction that significantly modulates the catalytic activities in either acidic or alkaline HER, highly efficient HER electrocatalyst through a self-gating phenomenon induced by Pt single atoms (SAs) anchored ultrathin NiO nanosheets (NiO-Pt) etc.

Iridium-free anodes for proton-exchange water electrolysis

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The most technologically advanced water electrolysis (WE) technology for the generation of hydrogen from renewables uses proton-exchange membrane (PEM) electrolytes and presents many important advantages over the devices with traditional alkaline electrolyte systems. One major limitation of the PEMWEs is in the requirement for the use of iridium-based catalysts at the anodes that facilitate the oxygen evolution reaction (OER) at low pH and elevated temperatures. Apart from the impractically high cost of iridium, the very low level of the production of this metal, viz. only few tonnes per annum, presents an essentially unsurmountable impediment to the implementation of the PEMWE technology on a multi-gigawatt scale.

Over the past years, we aimed to resolve the above challenge through the development of the iridium-free, earth-abundant OER catalysts that are capable of robust operation under acidic conditions and practical temperatures on an extended timescale. Our design strategy uses a so-called “catalyst-in-matrix” concept, viz. combination of an OER catalytically active species, like cobalt or manganese oxides, with an electrically conductive matrix that is thermodynamically stable under the operating conditions, like oxides of lead, antimony and bismuth.

The talk will highlight a range of the systems using different “catalyst” and “matrix” combinations and will provide insights into the modes of their operation, in particular those derived from the advanced electrochemical and in situ spectroelectrochemical studies. Finally, integration of the most promising earth-abundant OER catalytic system into the low-pH water electrolysis prototypes will be demonstrated.

Kinetic Analysis of Zinc Metal Production Using Low Concentration Hydrogen

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Electric arc furnace dust (EAFD) as a by-product from steel manufacturing has been considered to be hazardous waste. Amongst the various compounds, zinc oxide and zinc ferrite are the most commonly found within the EAFD. In this project, we have studied the process of zinc oxide reduction reaction using low concentration of hydrogen.

The kinetics of reduction reaction was analysed at different temperatures using both thermogravimetric analyser (TGA) and the tube furnace. The experiment at 500°C did not show any reduction at all. When the temperature increases from 750°C to 1100°C, the reaction rates against temperature showed a clear exponential trend. Advanced materials characterisation, including XRD, SEM and TEM, have been used to confirm the presence of Zinc metal after treatment.

Learning from 100 papers: Challenges and Trends for Distributed Hydrogen Systems

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The global energy landscape is undergoing a significant transformation, focusing on low-emission hydrogen to decarbonize sectors with hard-abate emissions. The conventional structure of the fossil fuel energy supply chain is centralized. A potential alternative to the prevalent large-size centralized system of energy supply is the decentralized small-scale production closer to end-users, capable of producing electricity, heat, and secondary energy carriers like hydrogen. This study presents the current status and trajectory of distributed hydrogen systems based on a literature review of 100 published papers.

The extraction of scientific literature on distributed hydrogen systems is carried out on the Web of Science and ScienceDirect databases with keywords focused on renewables and green hydrogen production. Selected papers are reviewed to collect and classify their information in a systematic approach. Extensive analysis is performed on systematized information to reveal the progress and trends of distributed hydrogen systems related to distributed hydrogen system technologies, applications, future roles, end-use sectors, cost estimations, and anticipated challenges.

The results of this study indicate that the end-use cases of distributed hydrogen systems are positioned in the less-tier segment of the hydrogen utilization hierarchy and misleading in guiding the energy transition pathway. Specific concentration on global North countries and the lack of a universally agreed definition of distributed hydrogen systems highlights limited development in this segment and the need to expand the research horizon to encapsulate multiple contexts and realities.

The Lack of maturity in building-level hydrogen systems is attributed to the profound impact of system costs at this scale. In addition to this, the presented information on prevalent hydrogen production, transportation, and storage technologies, levelized costs of distributed hydrogen, and overcoming methodologies of pressing challenges will play a vital role in advancing scientific understanding, knowledge dissemination, and progressing hydrogen research in the right direction.

Magnetocaloric properties of metal-substituted Ho-B alloys

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Magnetic refrigeration is a promising alternative to conventional refrigeration technology due to its energy efficiency, environmental friendliness, and higher cycle efficiency, particularly with potential application for hydrogen liquefaction. To develop and optimize magnetocaloric materials for this purpose, a wide range of materials with tuneable working temperatures and enhanced magnetic entropy is required.

We report on arc melt syntheses of metal-substituted (~10% of Fe, Sn or Nb) Ho-B alloys and characterisation of their magnetocaloric and microstructural properties. XRD data and microstructural analysis reveal that Sn does not substitute, and Fe shows limited substitution, into HoB₂ by this synthesis method; therefore, no significant changes to HoB₂ properties were observed for products with low, or no, levels of added Fe and Sn.

However, Nb addition results in substantive changes to unit cell parameters which suggest substitution to form the compound (Ho_{0.93}Nb_{0.07})B₂. Nb substitution results in an additional suite of alloys suited to magnetic refrigeration with enhanced Curie temperature and decreased magnetic entropy compared with HoB₂.

Mapping Formic Acid Oxidation across Platinum Grain Boundaries

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Decreasing carbon emissions remains as a global goal and is essential for the sustainability of current and future energy demands. Using electrochemical methods, formic acid can be oxidised and the energy utilised in fuel cells which is a promising step towards carbon neutrality. The electrochemical conversion of formic acid is limited by the efficiency and selectivity of the electrocatalysts on which the reaction happens. Platinum has been researched extensively for this application, although it has limitations due to surface poisoning.

Our aim is to quantify the relationship of the rate of electrochemical formic acid oxidation and the structure of a Platinum surface across different crystal orientations and grain boundaries. Scanning Electrochemical Cell Microscopy (SECCM) will be used to generate maps of the rate of electrochemical oxidation of formic acid over the Platinum grain boundaries with hundreds of nanometre resolution, revealing the location dependent changes in the formic acid oxidation reaction.

Mapping Nanobubble Nucleation during Oxygen Evolution

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Bubble formation is a problem that impacts the performance, activity, and efficiency of electrochemical reactions. Bubbles can adhere to and cover the surface of active electrocatalytic sites. However, it is very challenging to analyse and visualise the initial nucleation and growth of bubbles because of the nanoscale size of the bubbles at this stage.

We investigate individual gas bubble nucleation and dynamics using Scanning Electrochemical Cell Microscopy (SECCM). We focus on the electrogeneration of a single oxygen nanobubble during the Oxygen Evolution Reaction (OER) on nickel surfaces. We have found that single nanobubble reproducibly nucleates using 1 M KOH at ~1.35 V cyclic voltammetry (CV).

Our approach will allow us to map bubble nucleation on heterogeneous nickel surfaces with different facets or grain boundaries and nickel-based metal oxides with spinel structures AB_2O_4 to deepen the understanding of nanobubble behaviours further. Systematic investigation of interfacial nanobubble roles and behaviours will help develop nanobubble-based strategies to design high-performance electrocatalysts, especially using non-precious metals such as nickel or nickel oxides as the electrodes.

Mauri Model Decision Making Framework: how to incorporate measurement of Te Mauri O Te Wai and an appreciation of Infrastructure Belonging

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³Ngāti Porou

Iwi throughout Aotearoa have successfully challenged and reshaped the historic resource extraction processes of Colonial NZ across water, mineral and geothermal resources. Challenges through the Environment Court, where the quantification of impacts upon mauri has been adopted, have broadened the basis for infrastructure belonging. Changes have also resulted from Māori organisations, demonstrating the value of Indigenous epistemologies in improved resource management decision making.

Pūhiko Nukutū is investigating the conceptual belonging of a Green Hydrogen Industry in Aotearoa, while geographically explicit research is investigating the technical potential and feasibility of Green Hydrogen storage in Taranaki. The impacts that Green Hydrogen will have on Te Mauri o Te Wai is an essential consideration that will shape how this industry gains acceptance in Aotearoa. It is therefore important to increase awareness of underpinning concepts such as mauri and in particular investigate appropriate decision making processes that can effectively combine all relevant knowledge.

The Mauri Model Decision Making Framework is being applied to demonstration projects with four Iwi to socialise its use. Collaboration on a holistic analysis of Green Hydrogen technologies will follow. A project co-designed with Te Arawa Iwi is shared, and preliminary findings are discussed.

Flood gate infrastructure controls the movement of water from Rotoiti. Infrastructure belonging over the previous fifty years is analysed by considering the impacts on mauri and mauriora that have resulted from the flood gates. Cumulative impacts aligned to Te Mana o Te Wai hierarchy are considered.

Pūhiko Nukutū research outputs can inform the improvement of decision making processes strengthening the consideration of ecological and cultural priorities in the management of freshwater, and in turn, will also inform the applicability of Green Hydrogen technologies in Aotearoa New Zealand.

Mesoscale model for dissolution and coarsening of catalyst nanoparticles

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Power loss in polymer electrolyte membrane (PEM) fuel cells is mainly caused by the loss of the electrochemically active surface (ECSA) of the cathode catalyst layer. To investigate cathode aging, we developed a theoretical framework to study electrochemical dissolution of catalyst materials and predict nanoparticle coarsening over cycling.

A key feature of the proposed mesoscale approach is the explicit representation of the cathode catalyst microstructure and the local environment around each particle. Structure and environment are taken into account in modeling ions transport and the dissolution/redeposition processes caused by voltage cycling. In addition to capturing local effects, the model provides statistically averaged properties of coarsening ensembles that can be probed experimentally by ECSA measurements and electrochemical tests.

This theoretical framework can be used to understand how material design influences catalyst degradation, to improve material utilization and extend fuel-cell lifetime in long-haul vehicles.

Mesoscale Modeling of Microstructural Mechanisms of Materials Performance and Degradation in Hydrogen Storage and Production Systems

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Many of the biggest challenges in the hydrogen energy research are associated with the fact that the operation and degradation mechanisms of the associated materials often involve the complicated coupling of chemical/physical processes over vast ranges of multiple length and time scales.

These kinetic phenomena tend to occur at or near several types of solid/solid, solid/liquid, and solid/gas interfaces, which in turn play key roles in determining the overall performance of hydrogen production and storage processes. Essentially, these are collective dynamic processes of atomic/molecular species that determine the thermodynamics and kinetics of nano- or micro-level characteristics.

Moreover, the relevant processes are also strongly influenced by the associated microstructures of the operating materials. However, the lack of clear understanding of associated mechanisms and their impacts on hydrogen production and solid-state storage reactions has hampered the acceleration of materials discovery and development.

Therefore, it is obvious that several modeling approaches that cover different length and time scales ought to be properly integrated in order to comprehensively explore the underlying mesoscale science during the co-evolution of relevant chemical and materials processes. Mesoscale continuum modeling frameworks can provide a unified platform for integrating the necessary atomistic and continuum approaches.

In this talk, we present our integrated effort as part of the DOE Hydrogen Storage Materials—Advanced Research Consortium (HyMARC) and Hydrogen from Next-generation Electrolyzers of Water (H2NEW) towards the multiscale modeling of solid-state hydrogen storage and hydrogen production, respectively.

In particular, we will demonstrate our recent development of a comprehensive mesoscale modeling framework for assessing and quantifying the microstructural effects on materials performance and degradation in hydrogen storage and production systems. Representative case studies will be presented, including hydrogen/oxygen/thermal transport, mechanical responses, reaction-induced phase transformations in component materials for solid-state hydrogen storage and high-temperature electrolysis.

Metal Energy Carriers: using iron powder as hydrogen energy storage.

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The impact of hydrocarbons on climate change is well known, and hydrocarbons for energy generation and use must be quickly phased out. Hydrogen produced via renewable sources such as solar, wind or hydroelectric power, is an excellent candidate for green energy, however there are two main issues:

(1) storage and transport: pure hydrogen is flammable and explosive, and therefore requires either high pressures or very low temperatures to be effectively stored and transported. This leads to a loss of efficiency and many risks.

(2) non-constant generation: current sources of renewable energy are intermittent (e.g. solar panels at night) and seasonal (e.g. less solar power available during winter compared with summer). Thus a “buffer” is required to cover the times when generation of power is not possible. While pure hydrogen could be used as a short term buffer in small quantities, due to point (1) above, a different medium is required for longer term hydrogen storage and transport.

At the Technical University of Eindhoven in the Netherlands, we study the potential of iron powder to be used as a hydrogen storage medium. It has advantages over other carriers, with a small explosion risk (compared with pure hydrogen), being non-toxic (compared with ammonia) and abundant. The redox reaction of iron combustion and reduction allows the same powder to be reused almost indefinitely as an energy carrier, however many aspects of such repeated, systematic combustion of metal powders remain unknown. An overview will be given of various burners, designed to study and capture various aspects of iron combustion, and some results thereof.

Metal Hydride Systems for H₂ Compression

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As industry transitions to net zero, hydrogen (H₂) is gaining interest as a potential energy carrier. There are, however, challenges associated with replacing existing technologies and infrastructure with H₂-based alternatives. An example is provided in the report produced by the National Renewable Energy Agency (USA), which showed that approximately 2/3 of the cost of delivering H₂ at refuelling stations was due to the cost of compression. Domestic H₂ fuel cell electric vehicles (FCEVs) have storage tanks approaching 700 bar, which require pressure above 900 bar in refuelling stations.

Metal hydrides are metals or intermetallic compounds that react reversibly with H₂. They absorb low pressure H₂ at low temperature, and discharge at a high pressure when their temperature is raised, achieving compression. Metal hydride-based compressors use heat, rather than electricity, to achieve compression, leading to potentially lower compression costs, particularly where waste heat is available. Metal hydride compressors also have no moving parts, leading to lower operating costs and increased reliability compared to conventional mechanical compressors. Challenges include optimising heat transfer within the reactors, and optimal selection of suitable alloys for each stage of the compression for a given application.

CSIRO, in collaboration with Griffith University, are developing a prototype 2-stage metal hydride-based H₂ compressor. The aim is to compress H₂ from 10 to 350 bar using heat below 150 °C. The theory on alloy selection developed at Griffith University has been used to identify optimum alloys for each stage of the compressor. Reactor and pressure vessel design has been progressed at CSIRO, including novel methods for housing the alloys and improving heat transfer. This presentation will provide an overview of the research project and highlight recent progress in the design and commissioning of the prototype compressor.

Multi-Period Feasibility Study of Green Hydrogen Supply Network in Decarbonising New Zealand's Industries

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The production of green hydrogen and its derivatives is emerging as a strategic approach to achieve net-zero emissions while meeting energy and industrial demands. New Zealand is actively transitioning to increase its renewable energy share, seeking viable alternatives to gradually phase out fossil fuels. The government's legislation, banning offshore oil and gas exploration, not only strains energy security but also impacts key industrial products like fertilizers and various chemicals (e.g., methanol, DME, and other higher hydrocarbon fuels).

This presentation focuses on a macro-scale model for New Zealand's hydrogen economy, incorporating scenario-based macro-scale modelling across a multi-step period operation. The comprehensive green hydrogen supply network which will encompass renewable energy generation such as wind, solar and biomass, various electrolyzers, and storage and delivery options tailored to its end-user demands will be optimised using a mixed integer linear programming (MILP) model approach. It will be coupled with geographic information system (GIS) modelling which functions to identify suitable storage and renewable energy production sites that streamline the hydrogen supply network to its industrial demands. Moreover, GIS identifies suitable co-location sites for safety, excluding urban centres and protected areas.

As the hydrogen value chain is described using a cost function, the most economically efficient solutions will be obtained with the optimal selection of different hydrogen pathways. However, in situations where green hydrogen supply fails to meet the hydrogen demand, non-renewable hydrogen with carbon capture and storage (CCS) technology can be used to cater for the shortage in green hydrogen supply.

Multiple case studies will illustrate the potential hydrogen network within the projected timeline from 2030 to 2050. This analysis considers factors namely the cost reduction of electrolyzers, electricity prices, carbon pricing, and hydrogen incentives. Additionally, sensitivity analysis on the green hydrogen price is conducted to identify alternative hydrogen pathways generated from the optimisation model.

Multi-scale approach for deconvolution and quantification of the chemo-elastic energies within FeTi metal-hydride interphase from first principles.

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In the realm of materials science within the hydrogen sector, understanding the interphase boundary energy between a hydride and its parent matrix is crucial for modeling metal-hydride phase transformations and their influence on hydrogenation kinetics. In this investigation, we employ atomistic models and micromechanical analysis to deconvolute the chemical and elastic components of the interphase boundary energy within the FeTi metal-hydride system. We then use the analysis of their interplay to predict the most likely stable morphology of FeTi hydride precipitates.

Our approach involved the creation of atomistic models of the metal-hydride interface and the quantification of the chemical contribution of the interphase boundary energy by employing density functional theory (DFT) calculations together with the appropriate thermodynamic equations.

Subsequently, we delve into the elastic contribution to the interphase boundary energy and ascertain the habit plane of β -FeTiH formation. This determination is achieved by combining the aforementioned chemical contribution within micromechanical analysis, both derived through rigorous DFT calculations.

Our analysis unveils the progression in the development of the β -FeTiH phase, showing that, initially, it exhibits near-isotropic behavior that subsequently evolves towards growth along a specific direction tilted approximately 19° relative to the $(001)_\beta$ plane of the β -phase, which ultimately attains a habit plane parallel to the $(001)_\beta$ plane.

These findings offer valuable insights into the intricate interplay between chemical and elastic contributions to hydride formation. Such insights hold significant implications for the integration of micromechanics into phase field simulations of FeTi alloy hydrogenation—an ongoing focal point of research in our group.

Multiscale Modeling of Heterogeneous Interfaces for Hydrogen Production

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Improving performance of hydrogen production devices requires a detailed understanding of physicochemical processes at solid-gas and solid-liquid interfaces. However, probing behavior of these interfaces under working conditions remain a significant challenge for both simulations and experimental probes.

In this talk, I will provide an overview of our strategy for simulating heterogeneous interfaces within the HydroGEN Advanced Water Splitting Materials Consortium, ranging from first-principles calculations of chemical reactivity to machine learning approaches for accelerating theory-experiment integration and continuum methods for understanding microstructure effects.

In particular, I will discuss how computational models can be used to elucidate mechanisms of interface chemical reactions and mass transport, as well as the formation of new phases and their impacts on materials stability and performance. I will also show how simulations have been integrated with experimental probes, such as X-ray spectroscopy, to obtain new understanding of materials interfaces under operating conditions.

Finally, I will discuss how this understanding is being used to guide new strategies for improving materials functionality for hydrogen production.

Multiscale Modelling of Doped TiFe for Solid State Hydrogen Storage

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The establishment of a hydrogen economy is integral to reducing the global reliance on finite fossil fuels and intermittent non-conventional resources. A critical aspect of hydrogen-based energy systems is safe and effective hydrogen storage. Solid state hydrogen storage using metal hydrides offer notable advantages in volume and energy efficiency over gaseous or liquid forms. TiFeH is one such metal hydride that shows promising hydrogen storage properties. Aotearoa New Zealand has substantial deposits of titanomagnetite ore that contains Ti and Fe intermetallic compounds. However, in their natural form, they contain many impurities, leading to two questions:

1. How do these impurities impact the hydrogen storage behaviour of the materials?
2. Can these impurities be beneficial for hydrogen storage performance?
3. How 'pure' must the TiFe be for best performance in terms of production cost and utility?

These questions can be addressed only by understanding nanoscale processes in hydrogenation and dehydrogenation of the doped materials. Computational modelling can be used to understand the hydrogenation from the atomic to the mesoscale. However, existing computational models largely assume ideal compositions.

The focus here is the computational modelling of TiFe hydride with substitutional and interstitial impurities. This work involves multiscale modelling of the material using density functional theory (DFT) calculations for atomistic modelling and OpenCALPHAD for the thermodynamic modelling of phase diagrams as a function of temperature and composition. The objective is to generate a detailed phase model that can be used to predict the hydrogenation behaviour in the presence of selected impurities and help optimize the alloy composition and working conditions.

Nanomaterials for photoelectrochemical H₂ production

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Semiconductor nanomaterials hold the keys for efficient solar energy harvesting and conversion processes like photocatalysis and photoelectrochemical reactions.

In this talk, we will give a brief overview of our recent progress in designing semiconductor nanomaterials for photoelectrochemical energy conversion including solar hydrogen generation and low-cost solar cells.

In more details, we have been focusing on a few aspects; 1) photocatalysis mechanism, light harvesting, charge separation and transfer and surface reaction engineering of low-cost metal oxide based semiconductors including TiO₂, BiVO₄ as efficient photoelectrode for photoelectrochemical hydrogen production; 2) the working mechanism and stability improvement of perovskite quantum dots for high efficient solar cells; 3) The design of ultra-stable composites of perovskite-MOF with improved light emitting performance. The resultant material systems exhibited efficient photocatalytic performance and improved power conversion efficiency in solar cells, which underpin sustainable development of solar-energy conversion application.

Net Zero Housing – Green Hydrogen from Solar Roofing

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In response to recent NZ Government initiatives to tackle the climate crisis, the Emissions Reduction Plan and the NZ Net Zero Fund, this presentation will summarise recent developments at Manufacturing Systems Ltd to fabricate a range of unique products aimed at maximizing the capture of solar energy from a roof and conversion into green hydrogen. Essential to those efforts is a patented continuous production capability, which paves the way to the mass-production of multi-layered patterned polymer surfaces for applications in a range of high-value, high-tech products.

The presentation will outline the manufacturing process and discuss the benefits compared to the more conventional methods employed in polymer processing. This continues with an introduction to a novel building-integrated PV and Solar thermal roofing system developed by MSL spinout company FWave (FWaveroofting.com) that is UL-rated and capable of up to 50% conversion efficiency. The key features of the roofing system will be discussed in the context of competitor products.

With FWave demonstration roofs currently being installed in Japan and the USA, the output data shows that the installations meet the anticipated energy capture efficiencies. The presentation will then summarise a novel heterogeneous catalytic convertor with enhanced performance due to the three-dimensional electrode surfaces and the electrocatalytic splitting of water into hydrogen and oxygen.

NiFeP_x electrocatalyst: electrosynthesis, electro-activation, and applications in photo-electrocatalysis

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Renewable energy-driven electrosynthesis of fuels and commodity chemicals with water as the proton source, such as hydrogen, adiponitrile, and hexamethylenediamine, have been considered as the promising route to achieve a carbon-neutral economy.

Oxygen evolution reaction (OER) is notorious for its sluggish kinetics and presents as the kinetic bottleneck in these renewable energy-driven synthetic processes. Alkaline electrolytes are often used to enhance efficiency, but disposal of highly corrosive solutions is problematic, and accounts for most of the operating cost and carbon footprint. In the present contribution, we report on the facile preparation of nickel-iron-phosphide (NiFeP_x) modified electrodes with high performance towards OER and applicability for seawater splitting and electrosynthesis of adiponitrile.

The effects of electrode composition and electrosynthetic conditions on the OER activity of the prepared NiFeP_x electrode were thoroughly investigated, and the XAS analyses discovered the essential roles of P and Fe species played in enhancing the OER activity at neutral pH. In the case of seawater splitting, the activated NiFeP_x electrode shows high activity and stability under high turnover conditions, reaching 10 mA cm⁻² (turnover frequency: ~0.79 s⁻¹) at an overpotential of ~700 mV, with a moderate increase in η (~50 mV), mainly due to the change in local pH, over 15 h of electrolysis in phosphate-buffered (0.5 M, pH 7) seawater.

The integration of NiFeP_x onto the TiO₂ nanodendrite photoanode for photoelectrochemical seawater splitting is also demonstrated. On the other hand, the prepared NiFeP_x electrode maintained its high OER performance in the electrolyte solution, containing acrylonitrile, tetrabutylammonium phosphate, used for the industrial electrosynthesis of adiponitrile, whereas the benchmark IrO_x electrode degraded quickly with 10 min operation at the same condition.

Optimising the Transition to Hydrogen Trucks: A Fleet Replacement Strategy for New Zealand

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As New Zealand commits to a net-zero emission economy in 2050, researching the transition of heavy vehicle fleets to hydrogen power becomes increasingly pivotal.

This study explores the economic feasibility and strategic timing for replacing heavy-duty diesel trucks with hydrogen-fuelled alternatives.

A total cost of ownership (TCO) model for heavy-duty diesel trucks, including hydrogen vehicles, is constructed to inform fleet owners' replacement decisions.

The research analyses key factors influencing these decisions, including hydrogen costs, service demand, and vehicle pricing, through a comprehensive sensitivity analysis.

Our findings from a comparative TCO analysis between diesel and hydrogen trucks, utilising New Zealand vehicle data, have yielded an optimal replacement timeline.

Subsequently, a cost minimisation model for fleet operation is developed, considering annual evaluations to minimise TCO while fulfilling service demands and budget constraints for new truck acquisitions until 2035.

The methodology employs a sequential decision-making algorithm to determine the optimal fleet composition and replacement schedule, adjusting for the TCO of existing and new trucks.

This approach underlines the strategic importance of optimising fleet replacement to leverage the benefits of New Zealand's emerging hydrogen economy.

Overview of the U.S. DOE Hydrogen Production and Storage Consortia: A Computational Perspective

Wood B¹

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I will provide an overview of some key activities in three multi-laboratory hydrogen consortia funded by the U.S. Department of Energy: HydroGEN, focused on materials for renewable hydrogen production; HyMARC, focused on materials-based hydrogen storage and liquid hydrogen carriers; and H2NEW, focused on degradation and manufacturing challenges in high- and low-temperature water electrolyzers.

I will first discuss how these consortia fit into the overall landscape of hydrogen research within the U.S., including current and future priorities.

Next, I will emphasize the specific role of high-performance computing within these consortia, which is being used to simulate relevant chemical processes at solid-gas, solid-liquid, and solid-solid interfaces in hydrogen materials and components at a wide range of scales.

Examples will highlight the integration of ab-initio atomistic models, continuum microstructural models, and macroscopic device models to elucidate key mechanisms, guide materials design, and identify limiting factors for materials performance and durability under operation.

I will also highlight the importance of integrating high-performance computing with high-fidelity experimental characterization to obtain new understanding of interfacial phenomena and guide strategies for improvement.

Oxygen nanobubbles under confinement

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The efficiency in hydrogen production using Anion Exchange Membrane Water Electrolysers (AEMWEL) is a significant obstacle to its practical application.

During water electrolysis, oxygen gas (O₂) bubbles form on the anode electrocatalyst's surface, which increases the cell resistance, ultimately reducing energy efficiency.

Moreover, anode electrocatalysts are designed with a highly porous surface to reduce the oxygen evolution reaction's (OER) overpotential, which often results in nanobubbles forming in the narrow gaps between the catalyst particles. This porosity makes studying O₂ nanobubbles in such a scenario very challenging.

The aim of this research is to simplify and quantify the study of oxygen nanobubbles that result from the OER reaction on a non-noble metal (Ni-based) electrocatalyst. To achieve this, we are investigating how oxygen nanobubbles behave under confinement of the electrolyte in a precise lithography-patterned nanofluidic channel. By gaining insights into the behavior of O₂ nanobubbles in this setup, we can optimize anode catalyst and electrode structures to enhance AEMEL performance.

Pelletization and induration of New Zealand titanomagnetite ironsand for hydrogen direct reduction

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Hydrogen-direct-reduction (H₂-DR) of iron ore in a vertical shaft furnace is a promising zero-CO₂ ironmaking approach. This requires the pelletization of iron ore fines which then undergo induration at high temperatures to increase the pellet strength before it can be fed into the shaft furnace.

Here we report the pelletization, induration, and subsequent hydrogen reduction behaviour of New Zealand titanomagnetite ironsand. Initially, the effect of different ironsand particle size and induration conditions on the compressive strength of pellets bonded with bentonite and commercially sourced carboxymethyl-cellulose was studied.

Optimal strength was obtained through the formation of a liquid bonding phase at 1200°C. Organic binders like carboxymethyl-cellulose were found to effectively increase the green strength of pellets, whilst inorganic additives such as bentonite promoted the formation of a liquid bonding phase between particles during induration.

The pellets were then reduced with hydrogen gas in a thermogravimetric furnace at 1100°C, with all samples achieving a reduction degree of 97%.

This indicates that the different pelletisation procedures had little to no effect on the reducibility of pellets in hydrogen. Further tests are now focused on characterising the reduction behaviour of these pellets in a laboratory-scale continuous H₂-DR vertical shaft furnace.

Photo(electro)cduction by matching blue edge with absorptions the production of hydrogen and formate

Lai Y¹

¹National Cheng Kung University

Photo(electro)catalytic hydrogen production accompanied by organic waste valorization has been envisioned as an attractive strategy to tackle the global energy crisis and environmental pollution.

In the consideration of sustainability, our group aims to develop non-toxic and earth-abundant materials for photo(electro)chemical reforming organic waste to produce value-added chemicals and hydrogen. We found that monoclinic CuO (m-CuO) can act as a selective electrocatalyst for formate production from glucose and cellulose.[1] m-CuO can also be used as an efficient cocatalyst on a photoanode for photoelectrochemical glucose valorization. With m-CuO modification, the Faradaic efficiency for formate production of hematite can be enhanced from approximately 61% to nearly 100%.

In another study, we developed an efficient heterojunction g-C₃N₄/CuFeO₂ photocatalyst for hydrogen generation using plastic as a feedstock.[2] g-C₃N₄/CuFeO₂ shows much higher activity for solar-driven H₂ evolution compared to that of g-C₃N₄ and CuFeO₂ using hydrolyzed polyester microfiber as a feedstock, while the nuclear magnetic resonance analysis indicates that the primary organic product is formate.

These studies demonstrate that non-toxic and noble-metal-free CuO and g-C₃N₄/CuFeO₂ are efficient and selective catalysts for organic waste reforming.

[1] Selective production of formate over a CuO electrocatalyst by electrochemical and photoelectrochemical biomass valorisation. *Catal. Sci. Technol.*, 2022, 12, 6375-6383.

[2] Solar-driven hydrogen evolution in alkaline seawater over earth-abundant g-C₃N₄/CuFeO₂ heterojunction photocatalyst using microplastic as a feedstock. *Chem. Eng. J.*, 2023, 475, 146413.

Plasma Mediated Water Splitting for Hydrogen Production

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This mini-review explores the potential of enhancing hydrogen generation efficiency through plasma-based methods, with a focus on utilizing steam, and argon as a carrier gas. Various plasma generation methods, including dielectric barrier discharge (dbd), microwave, radiofrequency (rf), and gliding arc, exhibit comparable efficiency in hydrogen production, allowing for flexibility and adaptability in tuning the plasma and modifying reaction vessel parameters.

The integration of steam in plasma setups demonstrates a remarkable improvement in overall efficiency, ranging from 20-40% (relative to water), albeit incurring a mere 2% cost to the overall process converting water to steam.

Porous Materials for Organic Energy Storage Applications

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Organic energy storage systems, including batteries and capacitors, have undergone a renaissance in recent years due to humanity's transition towards a renewable and electrically powered world.

Typical energy-storage devices use heavy metals such as Cobalt, Nickel, and Manganese as cathodes, but these materials are difficult to mine and relatively rare making them expensive to scale up.

The discovery of highly porous materials such as porous-organic polymers, metal-organic frameworks, and covalent-organic frameworks, have allowed for the introduction of a new class of redox active porous energy storage materials which may aid in our energy transition.

Before the advent of these porous materials, organic functional groups could not be used as energy storage devices due to dissolution in the electrolyte.

However, the large size of these porous materials prevents the dissolution of organic functional groups allowing for utilisation in energy storage.

We have designed monomers for energy storage systems which utilise azo (-N=N-) functional groups through traditional, electrochemical, and microwave synthesis. Synthesised monomers were used in the fabrication of a porous energy storage material with a high specific capacity of 250 mAh/g.

Progress Towards the Ammonia - Hydrogen Economy

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Green ammonia has become widely recognized in recent years as a potential component of the future global energy economy. Produced from renewables, N₂ and hydrogen or water, ammonia can be viewed as an energy or hydrogen carrier.

As a hydrogen carrier it can be readily transformed catalytically into H₂ and N₂ at receiving port or point of use. It can also be used as a fuel directly in combustion engines, turbines and even co-firing along with other fuels. Of course, green ammonia also has an important role in displacing fossil fuel produced ammonia in the fertilizer and chemicals supply chains.

The traditional process for ammonia production uses H₂ and N₂ in a high temperature and pressure reaction that is capital intensive and usually only carried out at large scale plants that consume of the order of 1 GW continuously.

In our recent work we have demonstrated a direct electrolysis process that produces NH₃ at room temperature at high rates with faradaic efficiencies approaching 100%. Importantly, it has the potential to be implemented on a 1 – 100 MW scale appropriate to distributed installation at wind and solar farms.

This talk will review progress on the use of ammonia as a hydrogen carrier and fuel and the approaches to production at scale.

Rapid prototype screening of bipolar plate flow geometries for AEM water electrolyzers

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AEM water electrolysis leverages the advantages from both PEM and traditional alkaline electrolyzers. Unfortunately the performance of AEMELs lag behind PEM and alkaline electrolyzers due to the sluggish kinetics of the anode. Even at modest current densities (0.3 A/cm²), the anodic overpotential is above 250 mV, in contrast to 50 mV found at the cathode. To solve this challenge, our group are developing novel electrocatalytic materials.

In most laboratories, these type of electrocatalysts are tested in small 3-electrode cells. While these tests enable the inherent properties of electrocatalysts (surface area, catalytic activity) to be compared using a very simple and fast set-up, recent research [1] shows that translating electrocatalytic performance from 3-electrode cells to “real” AEM water electrolysis cells and stacks is not trivial, and in some cases materials with very different performance in 3-electrodes tests, perform very similarly in AEM cells. This highlights the importance of testing new catalytic materials under industrially relevant conditions.

It also suggests that there are factors in AEM cells such as electrolyte flow rate, gas bubble blocking, electrical resistances which are not found in 3-electrode cells but may actually influence performance in AEM cells, and thus in addition to optimising the catalytic material, the cell geometry (flow fields, porous transport layers, gas manifolds) and operating conditions (temperature, pressure, electrolyte concentration and flow rate) should also be optimised.

We have developed a 6-cell AEM stack which can operating at industrially relevant conditions and most importantly enables factors like cell geometry and operating conditions to be quickly changed to permit optimisation studies to be conducted.

In this poster, the influence of bipolar plate flow geometry and experimental conditions including electrolyte flow rate and conductivity, on the performance of the AEM stack is described along with the individual characterisation of each cell during operation.

[1] <https://pubs.acs.org/doi/10.1021/acsenergylett.2c01820>

Redox-mediated Electrocatalytic Nitrogen Reduction on a MOF Electrocatalyst for Green Ammonia Generation

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Ammonia is an important chemical to humankind – its use in fertilisers feeds billions of people. Unfortunately, industrial ammonia synthesis through the Haber-Bosch process is carbon-intensive, responsible for 1.3% of global emissions.

A promising alternative is to produce ammonia via the electrochemical nitrogen reduction reaction, where renewable electricity reduces nitrogen in water on an electrocatalyst. Metal-organic-frameworks (MOFs) are ideal electrocatalysts because they form 3D networks of active sites on which nitrogen reduction can occur. However, MOFs alone cannot achieve industrial ammonia production rates due to their poor electrical conductivity.

This research proposes the use of a redox mediator to shuttle electrons to the active sites of a MOF. Combined with a gas diffusion electrode to increase nitrogen transport, this novel system could achieve the highest ammonia production rate for MOF electrocatalysts. Such an electrocatalytic system could increase ammonia's viability in a hydrogen economy and could lead to a sustainable way to feed the world.

Reduction of iron-oxide fines using hydrogen

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Steelmaking is one of the biggest polluters of CO₂ in our current society. The main culprit for this is the chemical reduction of iron ores (iron-oxides) to pig iron (iron), which is currently almost entirely done using coal. Hydrogen can however also act as a reducing agent and, if renewable produced, it can significantly decrease our societies CO₂ emissions. However, the use of hydrogen instead of coal brings along quite some challenges: (1) the reaction kinetics are less well known, (2) hydrogen is known to increase the sintering of iron(-oxides), and (3) the reaction becomes endothermic instead of exothermic, requiring the rethinking of suitable reactors.

In this work, iron-oxide fines, produced by iron powder combustion, are used in various reactors to study the aspects mentioned above. The micron-sized spherical iron-oxide powder consists primarily of magnetite (Fe₃O₄) and hematite (Fe₂O₃). The reaction kinetics with hydrogen are studied in a thermogravimetric analysis, the sintering in a packed bed reactor, while a lab-scale fluidized bed is used to study the powder behavior in a more practical reactor. Results indicated that the reduction temperature has a strong influence on the morphology and sintering of the powders, while the hydrogen concentration has less of an influence. Above 600 degrees Celsius severe sintering occurs which prohibits proper fluidization.

Models have been developed based on the obtained results, which can be used to predict the reduction behavior, sintering strength, and minimum fluidization behavior.

Risk Communication and Public Acceptance of Hydrogen

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Risk communication has changed significantly in recent decades, moving away from one-way communication with the attempt to persuade citizens to change certain behaviour. This has shifted towards two-way communication with the idea of supporting citizens with fact-based knowledge so that they can make individual, knowledge-based decisions.

The production and use of hydrogen have so far been little aware of in households and in everyday life and is used more for industrial processes in Germany. As a result, there has been a lack of communication about the use of hydrogen and its potential risks. Nevertheless, it will be important in future to inform the public about the risks and potential uses, but also about the opportunities in dialogue with the public. The first newspaper articles about possible dangers have already been published in the media and these are being met with a poorly informed population and stakeholders.

Well-implemented risk communication does not mean greater social acceptance of hydrogen production or utilisation, but with openness, transparency and independent reporting it prevents the kind of misinformation that is increasingly appearing on social media. The higher the interest in the use of hydrogen, the more producers and users should think about successful risk communication on hydrogen. The presentation will show ways in which risk communication can be organised in the case of hydrogen use and on which factors social acceptance depends.

Ru-based catalysts for the proton exchange membrane water electrolyzers: The need to look beyond just another catalyst

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Water electrolysis provides a low-carbon route toward hydrogen production; however, it makes up only ~0.1 % of global hydrogen production. Apart from the significant capital and operating costs of green hydrogen through water electrolysis, the efficiency and rate of the core chemical process heavily depend on the availability of high-performance catalytic materials (Ir and Ir-based oxides) for the kinetically sluggish oxygen evolution reactions (OER) [1].

Ru-based electrocatalysts have attracted significant attention in academic and industrial communities due to their remarkably high activity in acidic electrolytes and lowest price in the noble metal family. Significant progress has been made in engineering Ru-based electrocatalysts, but an in-depth understanding of the engineering strategies and induced effects is still at an early stage.

Most recent research focuses on catalyst preparation via trial-and-error approaches and their evaluation at low currents. These catalysts possess a large degree of polydispersity and intrinsic heterogeneity; hence, any improvement in a specific parameter cannot be attributed to a specific change [2, 3].

In this work, we highlight that due to the intrinsic heterogeneity of the catalysts, any improvement in a specific parameter is a complex combination of various factors. Additionally, we propose ways to accelerate the understanding of the catalyst materials under operation and the development of large-scale water electrolyzers. A detailed discussion of recent literature and their characterisation will be given in the conference contribution.

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Synergistic Theoretical-Experimental Approaches in Metal Hydride Research for Solid-State Hydrogen Storage

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Metal hydride materials are a compelling avenue for the safe and efficient storage of hydrogen. Their exceptional volumetric densities surpass cryogenic alternatives, making them a critical component of a carbon-emission-free energy transition. Achieving this goal necessitates a profound understanding of the (de)hydrogenation thermodynamics and kinetics on different scales that underpin these materials.

The talk explores fundamental principles of hydrogen storage in metal hydride materials along with the current state of knowledge in this field together with the complexities and intricacies that this research faces.

To address these challenges, this talk will focus on shedding light on the collaborative synergy between theory and experiment at our research centre, providing insights into the latest advancements in metal hydride research for different application scenarios.

Synthesis of TiFe alloy for hydrogen storage applications by direct calciothermic reduction of ilmenite sand

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The transition to a hydrogen-based economy necessitates the exploration of safe, cost-effective energy carriers. The titanium iron (TiFe) intermetallic alloy stands out as a promising solid-state hydrogen carrier due to its non-toxicity, high volumetric density, and safety attributes, particularly for stationary applications. However, the conventional synthesis of TiFe relies on titanium and iron as raw materials, posing environmental and economic challenges associated with titanium extraction.

This study considers an alternative route to the production of TiFe through the direct reduction of ilmenite sand, an abundant natural resource, using calcium hydride (CaH₂) as a reducing agent. The reduction process was conducted in a tube furnace under an argon atmosphere, maintaining an ilmenite to CaH₂ mass ratio of 1:1.

Here we report a systematic exploration of the impact of temperature and time on this reduction process. Results indicate that a maximum TiFe yield of approximately 60 wt.% was achieved at 900°C after 1 hour of reduction.

For comparison, high-purity synthetic ilmenite was also reduced following the same approach, and this revealed a maximum TiFe yield of approximately 80 wt.%. These findings underscore the feasibility of metallothermic direct-reduction of ilmenite sand as an economically viable alternative to the conventional TiFe production route.

Synthesis, characterization, and properties of powder metallurgy transition metal-based high entropy alloys for electrocatalytic application

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Water electrolysis is an eco-friendly route for hydrogen production when compared to other routes such as steam reforming, coal gasification, biomass gasification etc, however only 4% of hydrogen is being produced through water electrolysis.

Water electrolysis proceeds via two half-cell reactions namely oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). HER is a two-electron transfer process while OER is a four electron/proton transfer process. Hence OER is energy intensive and affects the overall efficiency of water electrolysis. To improve the efficiency of water electrolysis, it is necessary to develop an efficient electrocatalyst for OER process. Ir and Ru based oxides are the state-of-the-art electrocatalysts for OER, however their natural abundance is minuscule, hence they are expensive.

Hence to overcome the shortcomings of conventional electrocatalysts a new class of multi component alloys termed as high entropy alloys (HEAs) are getting popular for electrocatalytic applications. However, most of the HEAs for OER are not self-supporting and being synthesised in powder form and are often coated onto conductive substrates such as Ni foam and carbon fibre.

In addition, most synthesised HEAs consist of Co which is an inherently expensive material. This research considered three Co free self-supporting HEA combinations namely NiMnFeCu, NiMnFeCrCu and NiMnFeCr which were successfully synthesized. Among the synthesized HEAs examined, NiMnFeCr was found to exhibit an overpotential of 300 mV after it was subjected to 100 cycles of cyclic voltammetry (CV) activation.

Furthermore, the NiMnFeCr HEA synthesised exhibited a compressive yield stress of 306 MPa manifesting the excellent combined properties of not only catalytic activity but also mechanical strength.

The research showed that NiMnFeCr was a suitable candidate material for industrial scale water electrolysis and hence can be considered as a potential replacement for the conventional, prominently used electrocatalysts such as Raney nickel, Ir and Ru oxide.

Te Mana O Te Wai: Relevance to a Potential Hydrogen Industry for Aotearoa NZ

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Almost fifty years on from the enactment of the Treaty of Waitangi (1975), Te Mana o Te Wai represents a conceptual shift towards including the underlying values of Tangata Whenua regarding freshwater. This enables greater respect towards water bodies and deprioritises water consumption for financial gain. Changes in policy and law now mean that mātauranga Māori and its accompanying ways of knowing must be included in decision making about freshwater in New Zealand. The new hierarchy places obligations on governance processes towards more highly valued ecological, social and cultural priorities in the management of freshwater.

The New Zealand Policy Statement for Freshwater Management (2020) has reframed our relationship with water. Te Mana o Te Wai describes a new hierarchy for the prioritisation of freshwater use. The first obligation is to the health and wellbeing of the river itself. Municipal water supplies are a lesser obligation, followed by other consumptive uses such as green hydrogen, and while also permitted, these uses cannot adversely impact the health and wellbeing of freshwater.

Within the New Zealand context, green hydrogen has rapidly established itself as a viable fossil fuel substitute and essential component of future energy scenarios. The scale of a hydrogen economy needed to underpin such a transition is however estimated to be 150 petajoules annually (First Gas, 2020). Hydrogen is produced using hydrolysis, a process best suited to freshwater, and the volumes of freshwater needed are significant at 13 million m³ annually.

Therefore the impacts of green hydrogen on the health and wellbeing of our freshwater, and how Te Mana o Te Wai hierarchy will be implemented, are essential matters that need to be thoroughly understood by our Hydrogen Industry. How these complex relationships can coexist will be a necessary focus of our research going forward.

Techno-economic feasibility of offshore wind farms for green hydrogen production: A case study from New Zealand

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As the demand for sustainable energy resources continues to rise, offshore wind farms have emerged as a promising solution due to their consistent and higher wind speeds in comparison to onshore wind farms. However, the substantial costs associated with infrastructure development have raised concerns.

This study explores the optimal setup of offshore wind farm facilities for generating green hydrogen, which offers a promising solution to address the intermittency of renewable energy sources and the challenges of long-distance energy transmission.

The approach used in this study is linear optimization, which aims to minimize the levelized cost of hydrogen (LCOH) by considering wind farm size and electrolyzer capacity as key decision variables.

This research investigates four distinct scenarios, all centered around the interplay between offshore wind power generation and green hydrogen production, both offshore and onshore. It aims to estimate and compare LCOH values under various wind energy configurations, specifically when offshore wind energy production either exceeds or falls short of the electrolyzer plant's capacity.

A case study is conducted, focusing on a proposed offshore wind farm to be built 22km off the coast of South Taranaki, New Zealand by the end of the decade.

The findings of the study highlight several key insights. Firstly, as onshore hydrogen storage capacity increases, LCOH decreases, particularly when offshore wind farms are situated closer to the coastline.

Furthermore, the LCOH for offshore green hydrogen production is notably lower compared to onshore production when the electrolyzer plant operates below its full capacity. Additionally, a sensitivity analysis involving various discount factors reveals their impact on reducing the LCOH over time.

In summary, this research offers valuable insights into optimizing offshore wind farms for green hydrogen production, considering different scenarios and their implications for the levelized cost of hydrogen, to support the transition to sustainable energy sources.

Testing of molecular catalysts for homo- and hetero-geneous HER and CO₂RR

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Current and past use of fossil fuels has led to the unsustainable warming of our climate.¹ The global warming crisis has highlighted the need for clean renewable energy sources to mitigate the ongoing damage. Catalysis of the hydrogen evolution reaction (HER) and CO₂ reduction reaction (CO₂RR) are pathways to be developed towards this goal.

The HER and CO₂RR are energetically demanding processes necessitating the development and testing of new catalysts to provide energy reduction, and selectivity of products in the case of CO₂RR.² Molecular catalysts provide the opportunity to tailor the selectivity towards specific products by fine tuning the molecular architecture.

A series of first row transition metal complexes have been tested for catalytic activity in the hydrogen evolution reaction (HER) and CO₂ reduction reaction (CO₂RR).^{3,4} The testing was carried out in both homogenous and heterogenous conditions, the heterogenous system involving the immobilisation of complexes onto a solid carbon support.⁵ The results of these studies will be presented and discussed, along with our plans to develop these studies further.

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The Role of (H₂-Diesel) Dual Fuel Heavy Vehicles in Decarbonizing Heavy Transport in New Zealand

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Despite heavy vehicles constituting only 4% of New Zealand's total fleet, they contribute to 25% of the country's road transport emissions. Hydrogen fuel cell vehicles powered by green hydrogen are promising alternatives for decarbonizing heavy transport.

However, their widespread adoption faces the challenge of both high capital cost and lack of fuel availability.

This study investigates the role of hydrogen-diesel dual fuel heavy vehicles as a means of accelerating the uptake of hydrogen fuel cell vehicles in New Zealand, using a system-dynamics model. A nested multinomial logit is used to model consumer choice behavior in new vehicle adoption, considering attributes such as fuel availability and vehicle capital cost.

Due to their lower capital cost and their flexibility to operate on 100% diesel when hydrogen is unavailable, hydrogen-diesel dual fuel vehicles have the potential to grow rapidly and stimulate the growth in hydrogen refueling stations.

The study's results reveal that the uptake of hydrogen-diesel dual fuel vehicles over the next decade significantly enhances fuel availability for all types of hydrogen vehicles, thereby accelerating the timeline to achieve the minimum fuel availability required for widespread adoption.

The Role of Interfaces in Ionomer-based Water Electrolysis

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As electrochemical technologies become increasingly important in our energy paradigm, especially hydrogen, there is a need to examine them holistically.

Furthermore, for such technologies to become practical, they need to operate at high current densities to minimize various cell costs. This operating space necessitates the need for efficient transport of reactants and removal of products from the reaction site and in a solid-state architecture that utilizes ion-conducting polymers (ionomers).

Thus, the critical component is the charged interface where the reactions occur, whether electrochemical or phase transformation. In this talk, we will explore the various electrochemical interfaces in electrolyzers with a focus on describing the underlying physical phenomena and their inherent tradeoffs in terms of performance and durability.

Such tradeoffs are quantified through multiphysics modeling and key diagnostics of the cells including breakdowns of the various limiting phenomena at both the micro and macroscales, where the local conditions and environment around the reaction site impact reactivity.

We will also discuss the impact of interfaces and interfacial resistance on transport phenomena into the ionomers from the environment and ways in which they control and limit fuel-cell performance.

Finally, other interfaces within electrolyzers are critical including those between the catalyst layer and porous-transport layer. We will discuss how controlling the interfacial properties of the porous-transport layer through a subtractive method, namely, laser ablation, improves overall performance, especially with thinner catalyst layers and ultra-low loadings.

Titanate photocatalyst/polyurethane foam composite for facile biohydrogen production via photo fermentation from corn stover

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Because of its short gas production cycle, environmental friendliness, and ability to use abundant and renewable biomass as a raw material, biohydrogen production via catalyst-assisted photo-fermentation is an appealing strategy.

However, because powder or particle-based photocatalysts are soluble in water, the recycling process is time-consuming, inefficient, and environmentally hazardous. Thus, photocatalysts are typically used by immobilizing them on various nanoparticles (such as silica particles, magnetic nanoparticles, and so on) or filtration membranes.

The former involves complex synthetic procedures and necessitates centrifugation techniques/a strong magnet for recycling, whereas the latter necessitates a large amount of energy due to high mass transfer resistance.

To address this problem, we proposed immobilizing titanate photocatalysts (MgTiO_3) onto polyurethane foam (PUF). Using HAU-M1 bacterium and corn stover as a substrate, the developed MgTiO_3 @PUF composite demonstrated excellent H_2 production performance, with a maximum yield of 563 mL per gram of sponge and a very high energy conversion efficiency of 36%. Furthermore, with a negligible decrease in H_2 production efficiency, the MgTiO_3 @PUF photocatalyst can be successfully regenerated and reused for five cycles via simple squeezing.

Unlike filtration membranes, the developed foam-based catalyst has 3D interconnected large pores, resulting in negligible mass transfer resistance. Furthermore, the bulk structure of the foam makes the photocatalyst-foam composite easy to use and recycle without the use of a magnet or other energy inputs.

Because of its exceptionally high H_2 production efficiency, convenient operation, remarkable recyclability, and ease of separation, the obtained MgTiO_3 @PUF has enormous potential for H_2 production via photo-fermentation in real-world applications.

Transformation pathways towards a climate neutral European energy system using integrated power and gas networks

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The rapid and fundamental transformation of energy infrastructure towards climate neutrality poses significant challenges to both infrastructure planners and policy makers around the world. In order to make informed decisions, energy system optimization models play a fundamental role in assessing infrastructure needs under a variety of alternative scenarios for future development. These scenarios are based on current European targets for domestic production and import of hydrogen, and the associated uncertainty of availability and cost of green energy carriers in a global market.

To answer research questions on the optimal transformation pathway, we employ the energy system optimization model REMix for multi-period optimization with different carbon budgets and limited as well as perfect foresight. This integrated computation of transformation pathways allows us to derive a holistic strategy regarding both the least-cost transition and the optimal timing of infrastructure conversion from natural gas to hydrogen.

Due to the high spatial and temporal resolution required to adequately represent renewable energy sources and flexibility options, such models are among the largest linear optimization problems currently being tackled. This computational complexity is further increased by the integrated assessment across multiple sectors and energy carriers, and the integrated optimization along a multi-period transformation path to avoid stranded investments. To this end, some complexity reduction techniques such as myopic foresight and reduced time resolution are applied to manage the resulting complexity.

This presentation discusses insights and key findings from an integrated analysis of optimal transformation paths. First, we assess the required European energy infrastructure in terms of spatial allocation of generation capacity and robust network topology for both power grids and gas pipelines. Second, we explore the trade-off between annual investment rates in renewables and their impact on the remaining carbon budget of the European energy sector.

Unlocking the potential hydrogen storage in Taranaki Field, New Zealand: experimental program for Ahuroa cores

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To assess the feasibility of underground hydrogen storage (UHS) in the depleted hydrocarbon reservoir of Taranaki field, New Zealand, we provide an integrated laboratory study of geophysical, geochemical and geomechanical (3G) evaluation of the cores from Ahuroa-1 well. The Oligocene Tariki Sandstone is sampled at about 3km in depth. The mineralogy is 60-70% quartz, 6-15% Feldspar, 7-10% calcite, 5-8% Clay, and 1-2% of heavy minerals.

The laboratory program includes core-flooding (short-term) and aging (long-term) experiments. H₂ flooding will be characterized via capillary pressure and relative permeability, monitored with NMR experiments. Before and after H₂ injection and long-term aging experiments will focus on the potential changes in porosity and permeability, minerals and pore space based on micro-scaled Computed Tomography and Scanning Electron Microscopy, and static and dynamic elastic properties subjected to triaxial and nano-indentation experiments.

The preliminary results indicates that the Ahuroa-1 cores exhibit a porosity in the range 14.2% to 15.4% (13.9% to 15%), and gas permeability ranges from 24 to 233 md (23 to 228 md) within the confinement of 1-10 MPa. The reason for this significant variability in permeability is calcite cement. The static and dynamic Young's Moduli are similar for both samples, on average 13.5 and 16.3 GPa, respectively. Static and dynamic Poisson's Ratio are 0.12 and 0.16, respectively. The Indentation Modulus (M) exhibits contrast value from 17.3 to 29 GPa.

Notably, these elastic parameters exhibit a qualitatively analogous trend among the four cores, which helps to verify our measuring techniques.

The preliminary results based on the clean samples will be compared to that of the hydrogen reacted one. The result of this study would provide a useful data set, and demonstrate if the alteration of 3G properties could be contributed to development of this particular sandstone for UHS in the Taranaki basin.

Utilization of green hydrogen to drive a sustainable zero-emission wastewater denitrification process

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Nitrate pollution is a pressing concern globally, with considerable adverse consequences on the environment and human well-being. Current large-scale nitrate removal (denitrification) technology, known as heterotrophic denitrification, employed in wastewater treatment results in carbon dioxide (CO₂) and nitrous oxide (N₂O) emissions. N₂O is an extremely potent greenhouse gas (GHG) with a global warming equivalent of 298 times that of CO₂. Additionally, a significant amount of energy is consumed recycling nitrate-laden wastewater to conduct pre-anoxic denitrification. Thus, there is a strong desire to develop a sustainable zero-emission denitrification process, in alignment with New Zealand's Net Zero Carbon Act.

Hydrogenotrophic denitrification is a promising zero-emission approach for efficient nitrate removal from organic carbon-deficient waters, e.g., groundwater or secondary treated wastewater. This process uses hydrogen (H₂)-oxidizing autotrophic bacteria to reduce nitrate to dinitrogen gas (N₂), with previous studies indicating that it can significantly reduce denitrification-related direct and indirect GHG emissions. Furthermore, rather than producing CO₂, CO₂ is used as the sole carbon source by the H₂-utilizing bacteria. However, technical challenges such as low water solubility and the explosive nature of H₂ have hindered the application of this novel denitrification technology.

This research aims to develop a robust and efficient denitrification process using green-H₂ to minimize N₂O emissions and eliminate energy consumption in wastewater recirculation. Results from bench-scale experiments using an innovative 20-liter membrane biofilm reactor (MBfR) demonstrated its ability to effectively overcome low H₂ solubility, providing H₂ safely via bubbleless direct diffusion into a denitrifying biofilm.

Our findings highlighted the ubiquity of indigenous hydrogenotrophic bacteria in three of Auckland's main wastewater treatment plants and their ability to self-seed an efficient denitrifying MBfR. Our novel denitrification process could achieve a peak nitrogen removal percentage of 99.3% at a specific removal rate of 367.7 mg N/m²·d.

Utilization of LaNi₅ as a long-term hydrogen storage material for space applications

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The LaNi₅ intermetallic compound offers an appealing option as a hydrogen storage material for space applications owing to the high volumetric storage capacity, easy activation, and safety aspects. However, the material may be exposed to distinct kinds of radiation in a space environment which could lead to deterioration and thus negatively impact the performance over time. Hence, in this work we have investigated the long-term stability of LaNi₅ and its hydride phases when exposed to low-energy ionizing radiation by employing a combination of density functional theory (DFT) and molecular dynamics (MD) calculations.

The threshold displacement energies to form stable defects were calculated in high-symmetry lattice directions of the alloy phases with ab-initio assisted molecular dynamics. MD simulations with the possible damage energies also provided valuable insights on the primary damage events. The mechanism of defect formations, energetics, and the impact of defects on the electronic structure and stability were studied.

The complexity and computational cost of the calculations were reduced by training a machine-learned (ML) interatomic potential and thereby coupling large-scale MD with ab-initio methods.

This work further contributes a fundamental understanding of radiation tolerance and the subsequent suitability of LaNi₅ alloys for hydrogen storage under the harsh conditions in space.

Utilizing Synchrotron Radiation for Insights into Catalyst Behavior during Operation

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The central objective of achieving net-zero CO₂ emissions by 2050 relies on the capacity to convert renewable energy into storable fuels. Hydrogen plays a pivotal role in bridging the gap between renewable energy sources and end-users. However, the challenge of achieving cost-effective, widespread hydrogen production is a multifaceted endeavor.

This necessitates a deep understanding of electrocatalysis for the development of efficient catalysts. Current electrocatalysis research predominantly focuses on comprehending the changes that occur on catalyst surfaces.

To gain insights into how solid-liquid interfaces affect electrochemical processes, it is essential to analyze the surface chemistry at the point where the electrode and electrolyte meet.

In this presentation, I will illustrate how the NSRRC beamlines can provide this vital information. Our experimental findings highlight the valuable perspectives offered by in-situ/operando X-ray characterization in unraveling the true mechanisms governing catalytic reactions.

[1] Peng, C.K.; Lin, Y.C.; Chiang, C.L.; Qian, Z.; Huang, Y.C.; Dong, C.L.; Li, J.F.; Chen, C.T.; Hu, Z.; Chen, S.Y.; Lin, Y.G.; Zhang-Rice singlets state formed by two-step oxidation for triggering water oxidation under operando conditions. *Nature Communications*, 2023, 14, 529.

[2] Lim, S.C.; Chiang, C.L.; Peng, C.K.; Wu, W.B.; Lin, Y.C.; Lin, Y.R.; Chen, C.L.; Lin, Y.G.; Realizing the bifunctional electrocatalysis via local charge rearrangement of α -CrOOH-modulated Co@CoMoOx for overall water splitting. *Chemical Engineering Journal*, 2023, 452, 139715.

[3] Li, Y.; Peng, C.K.; Hu, H.; Chen, S.Y.; Choi, J.; Lin, Y.G.; Lee, J.M.; Interstitial boron-triggered electron-deficient Os aerogels for enhanced pH-universal hydrogen evolution. *Nature Communications*, 2022, 13, 1143.

[4] Lin, Y.C.; Peng, C.K.; Lim, S.C.; Chen, C.L.; Nguyễn, T.N.; Wang, T.T.; Lin, M.C.; Hsu, Y.J.; Chen, S.Y.; Lin, Y.G.; Tailoring the Surface Oxygen Engineering of a Carbon-Quantum-Dot-Sensitized ZnO@H-ZnO_{1-x} Multijunction toward Efficient Charge Dynamics and Photoactivity Enhancement. *Applied Catalysis B: Environmental*, 2021, 285, 119846.

Are we fully utilizing our proton exchange membrane water electrolyser?

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The compact design of Proton Exchange Membrane Water Electrolysers (PEMWEs) makes it difficult to in-situ study the current density, temperature, and oxygen distribution.

Therefore, a three-dimensional, steady-state simulation model has been developed to study these principles. The model scope includes a repeating periodic segment of the PEMWE anode half cell at the microscale consisting of a stainless steel 304 bipolar plate with flow channel ribs, a titanium-based mesh Gas Diffusion Layer (GDL), liquid water flow channels, and iridium oxide Catalyst Layer (CL).

The study focus is on the localised current density distribution and oxygen generation relationship within the CL, which with supporting literature, conclusions can be drawn on the activation overpotential, concentration overpotential, and overall cell efficiency. The membrane and hydrogen generation are not modelled as the study focus is the Oxygen Evolution Reaction (OER). A constant inward current density is applied with the electric ground set at the CL-membrane interface. A novel part of the model is the use of a geometrically defined GDL with pores allowing fluid flow.

The charge distribution throughout the entire half-cell was evaluated and it was revealed that the CL utilisation was roughly the same as the GDL porosity. Zero current regions within the CL are present below the GDL pores which results in zero active sites for reaction. Oxygen was generated under the solid regions of the GDL mesh where the current density was most concentrated and the oxygen spilled out from under the GDL, into the pores but only around the pore interior walls, and diffused into the flow channels.

Sensitivity analysis was performed which included manipulating the CL electrical conductivity, flow channel width, and applied current density which act as useful strategies to enhance catalyst utilisation. This work will form a basis to enhance PEMWE efficiency at the microscale.

Optimal Numerical Methods for Computational Fluids Dynamics Models of Proton Exchange Membrane Fuel Cells

Edwards H¹

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The performance of proton exchange membrane fuel cells (PEMFCs) is highly dependent on the internal distribution of their reactants (hydrogen and oxygen), water and heat. These can be difficult to study experimentally, requiring invasive specialised equipment. However, a well validated 3D computational fluids dynamics (CFD) model can predict the internal distributions, subverting the need for invasive equipment which has made dual experimental/computational studies popular in the literature.

Despite the frequency of modelling works in the literature, optimizing the numerical methods used in CFD PEMFC studies appears to be unexplored thus far. This is a common study performed in other areas of CFD study, so it would be of use for future PEMFC research to find which numerical methods are optimal in which operating conditions.

This study is performed using the Ansys Fluent PEMFC Addon Module, which is popular in the literature. The numerical domain consists of a small single channel model to perform the bulk of numerical methods comparisons, with the results confirmed on a 50 cm² full flow field. The pressure velocity coupling schemes and spatial discretization schemes are compared based on their stability, convergence rate, required computational resources and numerical accuracy. This is tested across several differing operating conditions, including high and low relative humidities and high and low temperatures.

Results indicate that the coupled method with pseudo-transience proved enhanced convergence and stability, making it well worth the computational resources. Second order upwind provides stability and accuracy. Higher order discretization schemes do not significantly improve accuracy. Regardless of the numerical methods, the model becomes unstable as the relative humidity exceeds 100% in the gas channels, requiring the under-relaxation of the channel liquid saturation. Additionally, these results are consistent on the 50 cm².

Green Hydrogen for Urban Energy Systems and Industries: Lessons from Germany

Alhamwi A¹

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Triggered by the European's Green Deal, the German government has made decisions that will lead to fundamental changes of the German energy supply systems.

Main goal is the integration of local renewable energies to decarbonize energy-intensive sectors using green hydrogen.

From a German perspective, this talk aims to highlight the role of green hydrogen for the decarbonization of energy-intensive sectors like industries and urban energy systems, its challenges and opportunities.

The production of green hydrogen and the extension of available gas networks in cities can support the transition towards a climate neutral urban energy system. "No Regret" strategy, however, should be followed for planning the development of urban hydrogen infrastructures.

Furthermore, a comparison of two case studies in Germany and New Zealand will be introduced.

A Molecular Dynamics Study of Interfacial Tension Between Gas Mixture of H₂ and Cushion Gas with Water Under Reservoir Condition: Implications for Underground Hydrogen Storage

Chang Q¹, Dempsey D¹

¹University of Canterbury

Hydrogen is projected to account for at least 10% of global energy in 20 years. The traditional cryogenic tank or vertical shaft may not be feasible for the storage of very large amounts of hydrogen. However, underground porous reservoirs with large storage volumes can accommodate larger-scale hydrogen production and provide sufficient capacity for managing out-of-phase supply and demand cycles.

The interfacial tension (IFT) between residual pore water and a gas mixture comprising H₂ and a cushion gas (e.g., CO₂ or CH₄) plays a key role in the distribution of injected gas and then the storage ability of H₂ in the reservoir. In this work, the interfacial tensions between gas mixtures of H₂ & CO₂, and H₂ & CH₄ with water were determined as a function of gas concentration at expected subsurface storage conditions of 20 MPa and 373 K.

In addition, an atomic-scale investigation of molecular behaviours at the gas-water interface, such as molecular adsorption, molecular orientation, and molecular mobility, was undertaken via molecular dynamics simulation.

Our goal was to determine the fundamental mechanisms of gas-water IFT evolution during underground hydrogen storage.

This work provides valuable insights into the molecular mechanisms underlying the impact of gas components on gas-water IFT, shedding light on the intricate dynamics at play in hydrogen storage in underground porous reservoirs.

Advancing Electrocatalysis: Impact of Morphology on Efficiency of Electrocatalytic Process

Hosseini A¹

¹CatalystTec

In the pursuit of cutting-edge devices for catalysis and energy conversion, the imperative lies in meticulous control of micro- and nano-scale surface functionalization. This study elevates the discourse by delving into the catalytic dynamics of flat surfaces vis-à-vis arrays adorned with micro-scale pyramids and nano-scale cones, revealing remarkable enhancements in conversion rates and localized thermodynamic shifts at precise tip apices.

Surprisingly, these shifts display a remarkable rigidity, challenging conventional expectations. Attributed to lowered pH at the tips, this phenomenon intensifies tip activity while dampening activity elsewhere. Leveraging current focusing at array tips, synergized with a self-assembled monolayer, imparts a heightened efficacy for selective functionalization. The subsequent diverse species functionalization further underscores the versatility of these approaches.

Our nuanced exploration not only propels the creation of spatially-selective and thermodynamically-efficient electrodes but also charts a course toward groundbreaking developments in electrochemical clean energy conversion systems, encompassing hydrogen and methanol fuel cells.

Solar Technology and Hydrogen Production: Exploring the Frontiers of Science

Duffy N¹, Yew R, Zahiri S, Kim J

¹CSIRO

In this talk, I will present the current status and approach to scalable hydrogen production that we are undertaking in the Solar Technologies Group at CSIRO. Our group is investigating a number of technologies for producing renewable hydrogen at scale.

Topics will include the use of photoelectrochemical water splitting to produce hydrogen using Bismuth Vanadate (BiVO_4) and the unique Cold Spray ZAP™ technology that utilises a solid state (melt-less) robotic additive technology that demonstrate a commercial advantage coupled with a small environmental footprint.

Results from our scalable BiVO_4 photoanode material will be presented along with a discussion on the ZAP technology used to produce Titanium photoanodes with high surface area and porosity, which enhances the light absorption and charge transfer efficiency.

The Solar technologies Group also maintains the only high-temperature solar thermal research facility of its type in Australia at the CSIRO Energy Centre in Newcastle. In Solar Field 1, the fine control of our Heliostats (sun-tracking mirrors) enables concentrated sunlight to be focused onto a target Photocatalytic reactor.

Whereas in Solar Field 2, we are developing a beam down reflector system for a pilot-scale 250 kW thermochemical hydrogen reactor. Initially, this facility will be used to generate hydrogen via the redox process, using ceria powder at temperatures of 1,100 to 1,400 °C. These technological approaches will be presented and have important implications for the development of sustainable hydrogen production.

How to Make Hydration of green hydrogen to drive a sustainable zero-emission wastewater denitrification process Efficient?

Meyer Q¹

¹University Of New South Wales

Low-cost, high-performance and durable hydrogen fuel cells are crucial for the success of the global hydrogen economy and Australia's hydrogen roadmap. Currently, researchers are attempting to reduce the reliance on scarce and expensive platinum by synthesizing low-cost alternatives using non-precious metals (such as Fe, Mn, Co). Fe–N–C structures containing Fe–Nx active sites are amongst the most promising platinum group metal-free catalysts for the oxygen reduction reaction.

However, despite narrowly closing the gap in half-wave potential in rotating disk electrodes over the last decade, their highest performances and durability are inferior to commercial Pt in real hydrogen fuel cells, suggesting device-level challenges.

In this talk, we shed light on this gap using the distribution of relaxation times and X-ray computed tomography to quantify the proton transport and oxygen reduction reaction kinetics of a high-performance Fe–N–C catalyst (1.08 W cm^{-2}) and a commercial platinum catalyst (1.7 W cm^{-2}) in hydrogen fuel cells.

Our work reveals that the slower proton transport and oxygen reduction reaction kinetics of Fe–N–C nanoporous carbon matrix considerably limits active site accessibility, unlike easily accessible Pt decorated on a carbon substrate.

We also investigated the catalyst degradations and discovered that after the loss of electrochemical active iron sites, carbon corrosion and ionomer degradation sharply reduce the catalyst layer utilization and cause a slow performance decay, with findings recently accepted in Energy and Environmental Science (in Press).

Furthermore, we introduced the largest super-resolved digital twin of the hydrogen fuel cell structure, allowing us to visualize large-scale (16 mm^2) water management challenges using Lattice-Boltzmann simulations [1].

This easily tuneable model will be crucial to further optimize the gas diffusion electrode and flow field structure to improve gas and water pathways to the active sites of high-loading non-precious metal catalysts.

[1] Nature Communications, <https://www.nature.com/articles/s41467-023-35973-8>

Energy-Efficient Catalysts for Green Ammonia Synthesis

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¹Liquium

Transitioning the “Hard-to-Abate” sectors like aviation, shipping, steel, cement, fertilisers towards zero CO₂ and greenhouse emissions has been extremely challenging. These sectors are the massive carbon emitters due to their enormous use of natural gases and crude fossil fuels.

Amongst them, ammonia, an essential ingredient for nitrogen-based fertiliser, is responsible for ~2% of total energy consumption. The science problem is that reacting nitrogen and hydrogen to form ammonia in the 115-year-old Haber-Bosch process is inefficient, energy-intensive, and requires high temperatures (>400°C) and pressure (>200 bar). Research to address these issues focuses primarily on reducing carbon emissions via alternative extraction methods for hydrogen, electrochemical ammonia synthesis, or catalyst developments, to cite but a few examples.

Despite several attempts, a simple catalyst material for widespread implementation of low-temperature/-pressure ammonia synthesis remains a challenge. In this presentation, we combine an experimental study with advanced computational investigations to show that lanthanide surfaces can break molecular nitrogen at ambient temperatures and pressures <1 bar with facile desorption – a remarkably simple catalyst approach that easily cleaves the strong nitrogen-nitrogen bond and more importantly releases the intermediate and final ammonia species.

In addition, key fundamental features, activation energy and reaction orders derived from experimental kinetic studies will be presented, highlighting the low activation energy as well as the reduced hydrogen poisoning of our lanthanide catalyst powders and pellets. Finally, computational investigations (ab initio molecular dynamics and density functional theory) to investigate the atomic-scale mechanism of the ammonia formation reaction will be discussed.

A multidisciplinary approach to unravel the geologic hydrogen system in the Yorke Peninsula, South Australia.

Bourdet J¹, Frery E¹, Sarout J¹, Markov J¹, Gong S¹, Delle Piane C¹, Strand J¹, Langhi L¹, Duque Nogueira Kiewiet M¹, Heath C¹

¹CSIRO Energy

Natural hydrogen as an energy source is a quickly evolving new frontier in the hydrogen rainbow with a Technology Readiness Level (TRL) comparable to green hydrogen. Natural hydrogen has been in production in Mali for the last 10 years and exploration is happening all over the globe with new discoveries being documented every month. As a matter of fact, the sector may be close to unlocking several other economical accumulations.

Research and method developments to investigate subsurface hydrogen is thus an active sector to support the pioneering industrial endeavour. At CSIRO, a multidisciplinary approach is being deployed in the South Australian Yorke Peninsula, linking the science of the seeps at surface, the geophysical data with what we can derive from investigating the rocks recovered at depth from drill holes.

For instance, we are developing workflows to measure the occurrence of hydrogen seeps at the earth surface in both dry and wet seasons, monitor the fluxes and track the origin of the leaky gases based on reliable gas detection, gas sampling, stable isotopes, and noble gases measurements. Basement and sedimentary cover cores provide data about the generation and retention potential. Furthermore, they contain record of the paleo-fluids that can be extracted and studied in-situ using microscopy-based methods to study the generation, migration, and fluid state of hydrogen and helium at depth.

Formulation and development of Oxygen Carriers for Hydrogen Production via Chemical Looping Processes

Nusheh M¹, Rosas S¹

¹Hot Lime Labs

The integration of chemical looping processes with pre-combustion methods, particularly steam gasification, presents an efficient and cost-effective CO₂ capture solution for renewable hydrogen production from biomass.

This innovative approach substitutes air in the fuel reactor with metal oxides, referred to as oxygen carriers, thereby enhancing energy efficiency and significantly lowering the marginal cost of CO₂ capture, a critical consideration for future mitigation scenarios. Moreover, the catalytic conversion effect facilitated by the presence of an oxygen carrier during steam reforming of gasification products, such as CH₄ or tar, contributes to increased H₂ yield.

Despite these advantages, the commercial adoption of this technology faces challenges related to durability, including issues like high attrition, agglomeration, coking, and reduced reactivity over multiple looping cycles. Addressing these concerns, Hot Lime Labs has developed solid oxygen carriers suitable for fluidized bed reactor systems. These carriers boast defined compositions, shapes, porosities, and sizes, crucial for optimizing transport and mixing. This not only impacts final productivity but also influences heat transfer and process control, thereby overcoming barriers to wider implementation in the industry.

Does the growing H₂ economy pose a risk to the environment?

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¹Materials Team, GNS Science

²Environmental Processes and Modelling, GNS Science

Concerns have been raised among climate scientists that emissions from the rapidly growing hydrogen economy may actually pose a risk to the climate that it is trying to protect. There are many unknowns related to the current concerns from hydrogen's short to long term atmospheric warming effects and leakage rates into the atmosphere from current and yet to be developed technologies. Furthermore, the estimated emissions range of 1-12% is also detrimental to the economics of the hydrogen economy.

Hence, GNS's Materials and Environmental Processes and Modelling teams are collaborating on a new project to consider and address these issues. The project will:

1. Review the current literature on direct/indirect atmospheric warming effects of H₂ emissions and synthesize it for NZ stakeholders.
2. Identify what emissions rates actually are from various hydrogen technologies (including generation, transport, storage, and usage), and identify how emissions could be mitigated.

The lack of empirical data, and growing concerns have the potential to stifle the development and uptake of H₂ technologies that will reduce our reliance on carbon-based energy. By better understanding this problem and how to mitigate it, we can prevent unintended consequences of these new technologies and increase support for a shift to a green hydrogen economy.

Advancing the Critical Role of Underground Hydrogen Storage in the Energy Transition

Sutton J¹

¹Lochard Energy

The global energy transition is well underway and with Australia's target of net-zero emissions by 2050, significant technological advances will be required to provide energy to support the supply security and stability (firming) challenges associated with renewable energy. Underground hydrogen storage (UHS) is considered a complementary technology and storage method alongside variable renewable energy generation.

Lochard Energy has completed a desktop study to consider the feasibility of underground hydrogen storage in the Waarre formation in the Onshore Otway Basin in Victoria, Australia. The study is holistic in considering the full life cycle of hydrogen production, through to storage and subsequent withdrawal and use, with the main technical focus being the subsurface aspects of underground hydrogen storage.

With a tremendous need for pilot demonstration projects to confirm the feasibility of UHS technology prior to investment in large-scale commercial operations, Lochard Energy has also designed a multi-criteria assessment methodology to identify and select optimal reservoirs within the Onshore Otway basin and associated sites for a UHS pilot demonstration project. In addition to the subsurface, surface factors such as land, road and power access and water availability have been considered. Importantly, non-technical, economic and social aspects such as community sentiment, regulatory and permitting requirements are also included.

This methodology provides selection options which enhance the probability of proving UHS viability and improves confidence in knowledge transferability to other fields within the basin. Lochard Energy's vision is that a successful pilot demonstration, combined with regulatory support and other factors, will ultimately enable commercial-scale development of underground hydrogen storage.

It is hoped that this method of energy storage will complement and enable further developments in the renewable energy space, and support the achievement of Australia's net-zero emissions target through multiple, diverse technological advancements.

Modular microfluidic fuel cell platform based on Lego-on-a-disc

Peter Kovalsky¹

¹The University of Waikato

Our newly created microfluidic platform called SPIN is the most recent creation of our research group. It is the amalgamation of Lab-on-Lego and Lab-on-a-CD. SPIN allows us to create chemical processes of moderate complexity at a modular microscopic scale. Centrifugal force provided by the spin drives the fluid from the feed reservoir to the receiving reservoir thus overcoming the necessity of precision dosing pumps. The example design shown in this work is a fully self-contained hydrogen fuel cell system comprised of a microreactor (chemical hydrogen generator) and PEM fuel cell stack contained within the cross-section of a single Lego row. For demonstration purposes, the fuel cell is connected to a Buck Boost converter to power a 1608 SMD LED thus illuminating at a threshold power of 50mW. The duration of the LED illumination during SPIN operation provides a simple indication of the total energy converted by the fuel cell. The modular nature of the Lego ecosystem provides an excellent framework for education and a low cost apparatus for demonstration of hydrogen storage and training in integrated hydrogen processes.

Nano-catalytic surfaces prepared by ion-implantation for electrocatalytic hydrogen evolution

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New Zealand's transition to a net zero-carbon economy requires effective transport and storage of renewable energy. Green hydrogen can fulfil the role of a zero-carbon energy vector with potential for long-term energy storage. In hydrogen production by electrolysis, water is split into oxygen and hydrogen gas via the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) respectively. With this process, electrical energy is converted to chemical energy i.e., chemical bonds of hydrogen. Currently platinum is the most effective electrocatalyst for the HER, however this noble metal is expensive. Transition metal carbides have the potential to be a low-cost alternative to platinum for HER. In particular, tungsten and molybdenum carbides are promising as they mimic the electronic properties of platinum.^{1,2}

Our research aims to overcome the barriers in synthesis of ultra-fine transition metal carbide nanoparticles by using ion beam methods. We use ion implantation techniques to synthesise nanostructured metal carbides at room temperature. Using X-ray photoelectron spectroscopy, ion beam analysis, atomic force microscopy and transmission electron microscopy, the properties of ion beam synthesized metal carbide nanoparticles are described. In addition, we will also present the electrocatalytic performance of these nanoparticles for hydrogen evolution reaction.

1. Kitchin, J.; Nørskov, J.; Barteau, M.; Chen, J., *Trends in the chemical properties of early transition metal carbide surfaces: A density functional study. Catalysis Today* 2005, 105, 66-73.

2. Wan, C.; Regmi, Y.; Leonard, B., *Multiple Phases of Molybdenum Carbide as Electrocatalysts for the Hydrogen Evolution Reaction. Angewandte Chemie International Edition* 2014, 53.

Novel Composite Monoliths for Hydrogen Storage

Hugh Davies (PhD student – Bath-Monash Global PhD programme)

(University of Bath supervisors) Prof. Tim Mays; Prof. Chris Bowen; Prof. Andrew Burrows

(Monash University supervisors) Assoc Prof. David Turner; Dr Parama Banerjee; Prof. Alan Chaffee

Physical adsorption of hydrogen gas in porous materials has attracted increasing attention in recent years due to its favourable adsorption/desorption kinetics, high gravimetric and volumetric capacity, low energy input and improved safety, compared to more conventional storage technologies such as high-pressure gas storage tanks and liquefaction.

High surface area adsorptive materials capable of high hydrogen gas uptake performance already exist, including activated carbons, metal organic frameworks (MOFs) and zeolites. However, these materials are typically used in their unconsolidated form in packed beds which presents handling and safety issues and limitations in parameters such as mass transfer. Processing unconsolidated adsorptive materials into monolithic forms mitigates these problems.

One method to process unconsolidated adsorbent filler materials is to bind them with a matrix. Matrices typically include materials such as clays and polymers which provide structural integrity but often significantly reduce active surface area by blocking or encapsulating the adsorbent filler material. Polymers of intrinsic microporosity (PIMs) are microporous materials, with BET surface areas around 700-800 m² g⁻¹. They are interesting materials as they can both provide structural integrity and, through their porous structure, can positively contribute to monolith surface area and adsorption capacity.

My research looks to develop novel nanoporous composite monoliths using a variety of ultra-high surface area fillers (BET > 2,000 m² g⁻¹) and PIM-1 matrix for hydrogen storage in sustainable energy applications. This has so far involved synthesising PIM-1, characterising the material using techniques such as Nuclear Magnetic Resonance (NMR), Gel Permeation Chromatography (GPC), and Thermogravimetric Analysis (TGA) as well as measuring nitrogen isotherms to calculate BET surface areas. Low pressure hydrogen isotherm measurements have also been carried out on the PIM-1 and some activated carbon fillers to understand their hydrogen storage capacities. Monoliths have been formed via freeze casting, a type of solvent casting used to form materials with structured porosity. The project will finetune freeze casting parameters with the aim of creating a methodology for the production of monoliths with replicable and controlled structures. The resulting monolith properties will be compared with those of their powdered material precursors and different monolith forms and structures will be investigated for optimisation of adsorption performance. Finally high pressure hydrogen adsorption isotherms will be carried out to simulate monolith adsorption capacity inside a hydrogen storage tank.

NSW Powerfuel including Hydrogen Network: a collaboration platform to accelerate Power-to-X innovation

Thomas Gao

The NSW Powerfuels Including Hydrogen Network within NSW Decarbonisation Innovation Hub is a transformative initiative by the NSW Government aimed at catalysing the development of renewable fuels within the state.

The network serves as a dynamic collaboration platform strategically designed to expedite Power-to-X (P2X) technology commercialisation and facilitate widespread industry deployment.

Thomas Gao's presentation will provide a comprehensive update on the network's key initiatives and outputs, showcase how the network's collaborative approach has fostered a thriving innovation ecosystem, serving as a model for accelerated P2X innovation in Australia and globally.

This presentation offers a unique opportunity to engage with the latest developments in the renewable fuels landscape and to explore potential avenues for collaboration within the network, its partners and members.