



ENERGY FUTURE CONFERENCE 2021

Virtual Conference

UNSW Sydney | 18 - 20 October 2021

Emerging Technologies across Hydrogen Value Chain

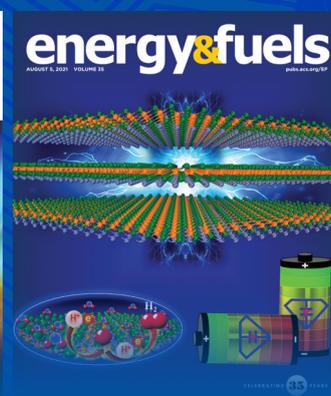
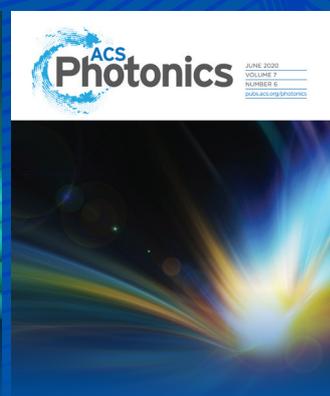
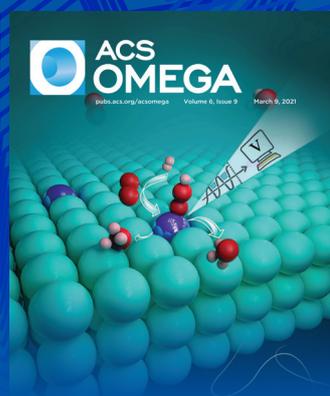
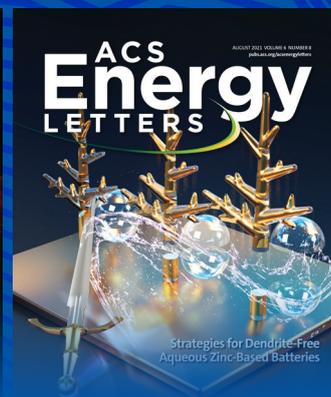
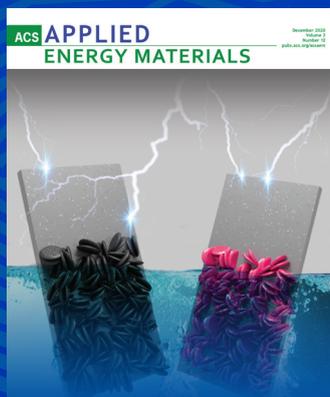


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FOREWORD

We would like to respectfully acknowledge the Local Indigenous people who are the Traditional Owners and Custodians of the land on which this meeting takes place.

Welcome to ‘virtual’ UNSW Australia and the 4th installment of the Energy Future Conference series, EF4 2021. We hope you all thoroughly enjoy all the event has to offer over the three days of talks, panel discussions and posters by the eminent academic and industry participants.

Since 2014, when the first Energy Future Conference was held, the mission of each installment has been to integrate and explore the diverse efforts in resources and approaches targeted at establishing renewable and sustainable energy technologies to maintain the momentum of Australian initiatives in the energy domain. As you are well aware, renewable hydrogen as an alternative clean energy vector is experiencing significant investment on both national and international stages where it is now viewed as a key energy contributor in the not-too-distant future. In light of this, the theme for EF4 2021 is “**Emerging Technologies Across the Hydrogen Value Chain**” where it will contemplate the entire hydrogen value chain including generation, storage, transport, transition/up-take, safety, application, social considerations, and the unseen challenges associated with each aspect.

As with past formats, EF4 2021 brings together academia and industry to disseminate and discuss expertise and experience in the hydrogen domain. The Conference will be officially opened by Mr Grant King, current Chairman of the Climate Change Authority, with days one and two having a technical focus, staging talks by national and international leaders in hydrogen research including plenaries by Prof Akihiko Kudo (TUS), Prof Anita Ho-Baillie (USyd), Prof Nate Lewis (Caltech), Prof Paolo Fornasiero (U Trieste) and Dr Fermin Cuevas (CNRS). The third day of the Conference will offer industry perceptions on hydrogen, beginning with an opening address by Prof Alan Finkel AO FAA FTSE, featuring industry-led talks and panel discussions on hydrogen policy and challenges with implementing hydrogen technology. The day will conclude with a HySupply panel discussion involving the Australian Ambassador Mr Phillip Green OAM, the German Ambassador Dr Thomas Fitschen, and HySupply teams from Germany and Australia exploring opportunities for renewable hydrogen for export.

The Conference itself is collectively hosted by the ARC Industrial Transformation Training Centre for the Global Hydrogen Economy, HySupply, the UNSW Global Water Institute, the ARC Research Hub for Integrated Energy Storage Solutions, the International Research Network: French-Australian Research Network on Conversion and Energy Storage (IRN-FACES) and UNSW Sydney and we would like to thank the help and support each of these entities has provided to help bring this event together.

We would also like to use this opportunity to sincerely thank all the sponsors of EF4 2021: NSW Department of Industry (sponsors since 2014) through the NSW Research Attraction and Acceleration Program Conference Sponsorship; ACS Publications (sponsors since 2018); and ProDigitek, Scitek, Shimadzu and Palmsens for their involvement and support. Finally, thank you to the Organising Committee, the Chairs, Panel Moderators, Poster Judges and EF4 volunteers and all the participants for their invaluable contributions (and their patience) which collectively will see EF4 2021 be an informative and knowledge-rich event. I hope you will enjoy EF4 2021 Conference and look forward to meeting you in Sydney, hopefully soon.



A/Prof Jason Scott

Chair of Energy Future 2021 Conference (EF4 2021)

ORGANISING COMMITTEE

- A/Prof. Jason Scott – Chair EF4 2021 & Co-Chairs of Technical Stream EF4 2021 (School of Chemical Engineering, UNSW Sydney)
- Dr Emma Lovell – Co-Chairs of Technical Stream EF4 2021 (School of Chemical Engineering, UNSW Sydney)
- Dr Rahman Daiyan – Co-Chairs of Industry Stream EF4 2021 (School of Chemical Engineering, UNSW Sydney)
- Prof. Greg Leslie - Co-Chairs of Industry Stream EF4 2021 (UNSW Global Water Institute & School of Chemical Engineering, UNSW Sydney)
- Scientia Prof. Rose Amal – Co-Founder EF Conference (School of Chemical Engineering, UNSW Sydney)
- Prof. Francois Aguey Zinsou Kondo - Co-Founder EF Conference (School of Chemical Engineering, UNSW Sydney)
- Ms Justine Jarvinen (UNSW Energy Institute)
- Ms Bridget de Pelleport (ARC Hub for Integrated Energy Storage)
- Dr Fermin Cuevas - CNRS Institut de Chimie et des Matériaux Paris Est (ICMPE)
- Dr Mandalena Hermawan – Conference Secretariat (School of Chemical Engineering, UNSW Sydney)

Plenary, Keynote and Invited Speakers Profile



Mr Grant King – Chair of Climate Change Authority and UNSW Energy Institute

Grant King retired after 16 years in his role as Managing Director, Origin Energy Limited, in October 2016. Grant has extensive experience in the Australian energy industry. He was formerly the Managing Director of Boral Energy and prior to that role, the General Manager, AGL Gas Companies where he held a number of management positions.

He is Chairman of HSBC Australia, CWP Renewables, GreenCollar and is Chairman of Sydney Water. He also Chairs the Climate Change Authority. He recently chaired the Expert Panel advising the Commonwealth Minister for Energy examining additional sources of low cost abatement and is currently a member of the Advisory Council for the Commonwealth Government's Technology Roadmap. He is also the Chairman of Arventa and runs his own advisory business specialising in energy markets, climate and technology. He also holds a position as Professor of Energy Engineering and is Chairman of the Energy Institute at the University of NSW. He is also a Director of O'Connell Street Associates. He served as President of the Business Council of Australia from November 2016-19. He is a former Director of BHP (April – August 2017), a former Chairman of Oil Company of Australia, a former Chairman of Contact Energy Limited and a former Director of Envestra Limited. He is also a former Director of the Australian Petroleum Production and Exploration Association Limited (APPEA), former Chairman of Energy Supply Association of Australia and former President of the Australian Gas Association.

Grant has a Degree in Civil Engineering from the University of New South Wales and a Masters of Management from the University of Wollongong. He is a Fellow of Australian Institute of Company Directors.

He is involved in a number of community and philanthropic activities. He is Chairman of the Melanoma Institute Australia, a Director of the Great Barrier Foundation and the Origin Energy Foundation and a member of the UNSW Foundation.



Professor Paolo Fornasiero – University of Trieste, Italy

Paolo Fornasiero is Full Professor in Inorganic Chemistry at the University of Trieste (Italy). His research focuses on the application of inorganic chemistry to nanoscience for the preparation of new materials useful in the fields of energy and environmental protection. He is co-author of about 250 publications on international journals, 15 book chapters and 4 patents. Since 2015 he serves as an Associate Editor of ACS Catalysis. He received the 2005 Nasini Gold Medal, the 2013 Chiusoli Gold Medal, the 2016 Heinz Heinemann Award, the 2017 Kramer Award and the 2018 M.T Messori Roncaglia Award.

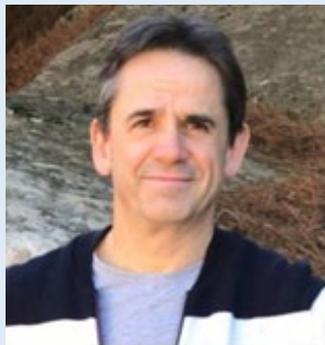
Title of talk: A personal perspective into the catalysts for hydrogen production



Professor Akihiko Kudo – Tokyo University of Science

Akihiko Kudo received his bachelor's degree from Tokyo University of Science in 1983 and his doctorate from Tokyo Institute of Technology in 1988. After a postdoctoral fellow at the University of Texas in Austin, he became a research associate at the Tokyo Institute of Technology until 1995. He then joined the Tokyo University of Science as a Lecturer before he became associate professor in 1998 and a full professor in 2003. Kudo received awards of the Japanese Photochemical Association in 2009, the 10th Green and Sustainable Chemistry from the Ministry of Environment in 2011, Catalysis Society of Japan in 2017, Academic Achievements in Ceramic Science and Technology in 2017, and Minister of Education, Culture, Sports, Science and Technology (2020). He was selected as a Clarivate Analytics Highly Cited Researcher in 2018-2019. His current research interest focuses on photocatalyst and photoelectrode materials for water splitting and CO₂ fixation of artificial photosynthesis.

Title of talk: Artificial photosynthesis using powdered photocatalyst materials



Dr Fermin Cuevas - East-Paris Institute of Chemistry and Materials

Fermin CUEVAS obtained his PhD in Physics at Autonomous University of Madrid (Spain) in 1996. After postdoctoral training at MPI Metals Research (Germany) and CNRS- East-Paris Institute of Chemistry and Materials (France), he got in 2002 a permanent research position at CNRS. His main research activities are focused on intermetallics, composites and complex hydrides for hydrogen storage as well as their functional properties as electrode and electrolyte materials for Ni-MH and Li-ion batteries. He has published over 150 articles in peer-reviewed international journals. He is currently head of the Interaction of Hydrogen and Matter group at ICMPE, co-head of the Storage axis at the French Research Network on Hydrogen Energy and French coordinator of the International Research Network on Conversion and Energy Storage for stand-alone & maritime applications

Title of talk: FeTi-based intermetallic compounds for large-scale stationary hydrogen storage



Professor Nate Lewis – California Institute of Technology (Caltech, USA)

Nathan S. Lewis, Ph.D., is the George L. Argyros Professor of Chemistry at the California Institute of Technology where he has been a faculty member since 1988. Lewis is best known for developing artificial photosynthesis technology that enables sustainable production of hydrogen fuel using sunlight, water and carbon dioxide. Research interests include the electronic nose that consists of chemically sensitive conducting polymer film capable of detecting and quantifying a broad variety of analytes. Additional research focuses on phototropism in non-biological inorganic matter and related pattern free nanoscale 3-D lithography. Lewis is also interested in weather-based data-driven modelling of deeply decarbonized electricity and energy systems based on variable renewable energy and technologies for long-term grid storage. From 2009 to 2019 he served as editor-in-chief of Energy and Environmental Science, a journal focusing on sustainable energy research, published by the Royal Society of Chemistry. He is the recipient of the Princeton Environmental Award and the American Chemical Society Award in Pure Chemistry. In 2019, he received the Europe Section Heinz Gerischer Award for his outstanding contribution to the science of semiconductor electrochemistry and photoelectrochemistry. In 2017, Lewis was elected to the National Academy of Inventors. He holds approximately 70 U.S. and foreign patents. Lewis has authored more than 500 papers and mentored more than 100 graduate students and postdoctoral researchers.

Title of talk: Sunlight-Driven Hydrogen Formation by Membrane-Supported Photoelectrochemical Water Splitting



Professor Anita Ho-Baillie – University of Sydney

Anita Ho-Baillie is the John Hooke Chair of Nanoscience at the University of Sydney, an Australian Research Council Future Fellow and an Adjunct Professor at University of New South Wales (UNSW). She completed her Bachelor of Engineering degree on a Co-op scholarship in 2001 and her PhD at UNSW in 2005. Her research interest is to engineer materials and devices at nanoscale for integrating solar cells onto all kinds of surfaces generating clean energy. She is a highly cited researcher in 2019 and 2020. She has been identified as one of the leaders in advancing perovskite solar cells. Her achievements in setting solar cell energy efficiency world records in various categories have placed her research at the forefront internationally.

Title of talk: By passing wires - Monolithic Integrated Devices for Solar Driven Hydrogen Production and Solar Batteries



Professor GJ 'Gus' Nathan – Centre for Energy Technology, University of Adelaide

Professor Nathan is the founding Director of The University of Adelaide's Centre for Energy Technology, Research Director for the Heavy Industry Low-carbon Transition CRC, a Fellow of the Combustion Institute, a recipient of a Discovery Outstanding Researcher Award from the Australian Research Council and an ATSE KH Sutherland medalist. He has led the development of 3 technology platforms to ongoing commercial use, including the ceremonial flame technology that was first implemented in the Relay Torch for the Sydney Olympic Games. He presently leads Solar Fuels program in the ARENA funded Australian Solar Thermal Research Institute and another ARENA funded program that is targeting cost-effective methods with which to implement up to 50% solar thermal energy into the Bayer alumina process. He has published some 300 papers in international journals, 250 peer reviewed conferences and 12 patents. He is a Fellow of the Combustion Institute, an ARC Discovery Outstanding Researcher, the inaugural AIE-SA Energy Professional of the Year

Title of talk: Emerging roles for hydrogen in decarbonising heavy industrial processes



Professor Evan Gray – Griffith University

Evan Gray has research interests focused on the physics of energy-related materials, including hydrogen storage materials and superconductors, and modelling energy systems. He has worked on materials for solid-state hydrogen storage for more than 30 years, using national and international neutron and synchrotron beam facilities to study structure-function relationships.

Evan manages the National Hydrogen Materials Reference Facility at Griffith University, which provides authoritative measurements of the uptake of hydrogen from ppm levels in high-strength steels to quantities for energy storage, at temperatures from cryogenic to 1000 Celsius, and hydrogen pressures from ultra-high vacuum to thousands of atmospheres.

Evan has a strong interest in the deployment of hydrogen-energy technologies in Australia. A focus on physics-based modelling of energy systems has developed around the pioneering Sir Samuel Griffith Centre, which incorporates hydrogen energy technology (electrolyser, metal-hydride hydrogen storage, fuel cell) to allow the building to operate off the electricity grid.

Title: Is there a role for metal-hydride hydrogen storage in the developing hydrogen economy?



Professor Lianzhou Wang – University of Queensland

Lianzhou Wang is Professor and ARC Laureate Fellow in School of Chemical Engineering, Director of Nanomaterials Centre, and Senior Group Leader of Australian Institute for Bioengineering and Nanotechnology, the University of Queensland. His research focuses on the design and application of functional semiconductor nanomaterials for renewable energy conversion/storage applications including new photocatalysts for solar hydrogen production, low-cost solar cells and rechargeable batteries. He has contributed 15 edited books and chapters, > 450 journal publications, receiving the citations of >30,000 times. He also won some prestigious Fellowships/awards including Australian Research Council (ARC) QEII Fellowship, Future Fellowship and Laureate Fellowship, UQ Research Excellence Award and Research Supervision Award, Scopus Young Researcher Award, and Research Excellence Award in Chemical Engineering. He is the fellow of Royal Society of Chemistry and is named in the list of the Clarivate' Highly Cited Researchers

Title of talk: Hybrid Perovskite Quantum Dots for High Efficiency Solar Cells



Professor Doug Macfarlane – Monash University

Doug MacFarlane is a Sir John Monash Distinguished Professor in the School of Chemistry, Monash University. Doug is head of the Energy Program in the ARC Centre of Excellence for Electromaterials Science. He is currently researching materials that will enable new pathways to generate energy and fuel from sustainable resources (e.g. the sun). One of his main focus areas within ACES is the generation of ‘Green Ammonia’ from nothing more than air, water and sunlight. He has published more than 800 papers and 30 patents and his awards include the Australian Academy of Science Craig Medal, and the Victoria Prize for Science and Innovation. Doug is also the Founder and Chief Scientific Officer of Jupiter Ionics P/L, a company spun out recently with seed funding from local investors to scale up the green ammonia generation technology developed in his group.

Title of talk: Towards Solar Fuels – Hydrogen and Ammonia



Professor Kylie Catchpole – Australian National University

Kylie Catchpole is Professor in the School of Engineering at the Australian National University. She has research interests in solar cells and solar fuels as well as the broader energy transition. Her group has achieved leading efficiencies for perovskite and perovskite/silicon tandem solar cells, and their work on direct solar-to-hydrogen generation was listed as one of the top 10 innovations by the Innovation for a Cool Earth Forum (ICEF) in 2020. She was awarded the inaugural John Booker Medal for Engineering Science from the Australian Academy of Science.

Title of talk: High Efficiency Direct Solar Hydrogen Generation



Professor Thomas Klassen – Institute of Materials Technology, Helmut Schmidt University and Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, German National Research Centre

Thomas Klassen is one of the pioneers in the field of nanocrystalline metal hydrides for hydrogen storage for more than 20 years, covering the full range from basic materials thermodynamics and kinetics to components and system integration. In addition, he is an expert for kinetic spray coating technology for more than 14 years, covering the basic mechanisms as well as application in nano-structured photoactive surfaces for hydrogen generation. Thomas Klassen has (co-)authored more than 285 peer-review papers (H-Factor 50) and over 20 patents, and he has presented 85 invited and keynote lectures. Currently, he holds a shared professorship as director of the Institute for Materials Technology at the Helmholtz-Zentrum Geesthacht (national research center) and as head of the Institute of Materials Technology at Helmut Schmidt University / University of the Federal Armed Forces Hamburg, Germany.

Title of talk: Hydrogen Generation and Storage: from Materials to Components



Dr Jessica Allen – University of Newcastle

Dr Jessica Allen is an electrochemical engineer and senior lecturer at the University of Newcastle in chemical and renewable energy engineering. Her research work spans electrochemical technology development including fuel cells and electrolysis as well as production of materials for batteries and other electrochemical energy storage systems. Dr Allen has published extensively in the field of molten salt thermochemistry and high temperature electrochemical reactions and is a well-known science communicator in the field of hydrogen energy, advocating strongly for a responsible energy transition in the Hunter region of NSW. Dr Allen is focused on the integration of renewable energy into industrial processes. As an ARC DECRA fellow, she is currently working on an innovative carbon capture and utilisation process which makes efficient and synergistic use of concentrated solar thermal energy through molten salt electrolysis.

Title of talk: Process considerations for electrochemically driven green ammonia and carbon negative materials



Dr Siva Karuturi – Australian National University

Dr. Siva Karuturi is currently working at the Australian National University (ANU), focussing on the development of semiconductor and catalytic materials for stand-alone solar hydrogen generation systems. He received a PhD degree in 2013 from Nanyang Technological University in Materials Science and Engineering. Siva worked as a postdoctoral fellow at the University of New South Wales (UNSW) in the School of Photovoltaics & Renewable Energy Engineering before moving to ANU in 2014. Siva was a recipient of the Discovery Early Career Researcher Award (DECRA) grant from the Australian Research Council (ARC) in 2015. Following this, he established a research program on solar water splitting research and has been involved in the training and supervision of 7 PhD students and several Masters by research and Honours students. His research been supported by grant funding from the Australian Renewable Energy Agency (ARENA) and Australian Research Council.

Title: Advanced Semiconductor and Catalytic Materials for Direct Solar Hydrogen Generation



Prof Umit Demirci – University of Montpellier

UBD received his PhD in physical chemistry in 2002 at the University of Strasbourg, France. After several professional experiences, he was recruited, in 2007, as associate professor at the University of Lyon I, France, focusing on hydrogen storage/generation, B-based materials, and catalysis. In 2011, he was transferred at the University of Montpellier, France. Since 2015, he is professor, still working on e.g. B- and N-based materials for hydrogen storage. He has also started a new research dedicated to amine boranes and materials for reversible H₂ storage. He (orcid 0000-0003-3616-1810) has co-authored more than 140 peer-reviewed papers. He is assistant editor for International Journal of Hydrogen Energy.

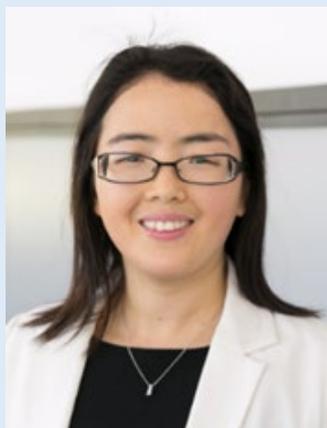
Title: MBNH materials for solid-state hydrogen storage – Focus on alkali and alkaline-earth hydrazinidoboranes



Prof Xiaojing Hao – School of Photovoltaic and Renewable Energy Engineering, UNSW Sydney.

Dr Xiaojing Hao obtained her PhD in the School of Photovoltaic and Renewable Energy Engineering (SPREE) of UNSW in 2010, and currently the Scientia Associate Professor at SPREE. A/Prof Hao has focused her research on low-cost, high-efficiency thin film solar cells and tandem solar cells for more than ten years, researching on various energy materials, initially using Si, and then earth-abundant compound semiconductor materials such as chalcogenide and perovskite for both solar photovoltaic and solar fuel applications. A/Prof Hao now leads a strong group in the above areas, achieving a number of efficiency records on emerging thin film solar cells. A/Prof Hao has published >150 peer-reviewed journal papers, including publications in Nature Energy, with several awards for her research excellence. She was the recipient of Inaugural ASI/ARENA Postdoc Fellow, previous ARC DECRA, and now ARC Future Fellow. She was awarded a number of prestigious national prizes, including 2020 Prime Minister's Prizes for Science: Malcolm McIntosh Prize for Physical Scientist of the Year, 2021 Australian Academy of Science Pawsey Medal.

Title: Design of Green Kesterite for Solar Photovoltaic and Photoelectrochemical CO₂ reduction



A/Prof. Yijiao Jiang – School of Engineering, Macquarie University

Dr Yijiao Jiang is an Associate Professor in the School of Engineering at Macquarie University (MQ) and the Chair of MQ Women in Engineering. After completing her PhD at University of Stuttgart, she worked as postdoc at ETH Zürich. She was then awarded UNSW VC Research Fellowship and ARC DECRA. Since joining at MQ in 2014, she has secured research grants from the ARC Industrial Transformation Research Hub with Rio Tinto and JITRI, ARC DPs, the EU Horizon 2020 etc. Her research interests focus on the development of better thermal-, photo-, and electro-catalytic systems for green chemical processes, renewable energy production and environmental remediation. She has developed various in situ and operando techniques including NMR, EPR, IR, Raman, and photoelectrochemical spectroscopy for catalysis research. She is an Associate Editor of Energy & Fuels and an Editorial Advisory Board Member of ACS Sustainable Chemistry & Engineering, Carbon Capture Science and Technology, and Scientific Reports.

Title: Heterogeneous Molecular Electrocatalysts for Carbon Dioxide Reduction in Water



Prof. Gunther Andersson – Flinders Institute for Nanoscale Science and Technology, Adelaide

In 1998 Gunther Andersson completed his PhD applying ion scattering spectroscopy on liquid surfaces at the University of Witten/Herdecke (Germany) under the supervision of Prof Harald Morgner. The following two years he was at the Technical University Eindhoven on a project on polymer-based light emitting diodes. In 2000 Gunther moved to Leipzig University (Germany) where he developed the method neutral impact collision ion scattering spectroscopy (NICISS) for investigation of soft matter surfaces to its current stage. He completed his Habilitation in 2006. In 2007 he was appointed at Flinders University (Australia). He is now leading as a full Professor a research group with activities in photocatalysis based on metal clusters on surfaces, and liquid and polymer surfaces and interfaces. His laboratories are equipped with instruments for electron spectroscopy (MIES, XPS, UPS, IPES), ion scattering spectroscopy (NICISS) and infrared spectroscopy (FTIR).

Title: Photocatalysts for H₂ Production Based on Metal Clusters as Co-Catalysts



A/Prof. Jonathan Love – Centre for Clean Energy Technology and Practises, Queensland University of Technology (QUT)

Dr Jonathan Love is an Associate Professor in the School of Chemistry and Physics at QUT. Jonathan has a PhD in Electrochemistry and 25 years RD&D experience in the international fuel cell industry. Jonathan joined QUT in 2018 to participate in the ARENA funded H2Xport project in the Centre for Clean Energy Technology and Practises. Jonathan's expertise includes fuel cells, electrolysers and the integration of science and engineering for prototyping, pilot plant construction and use, and manufacturing processes. Jonathan has researched with hydrogen for over 25 years and is currently involved in the design and build of an integrated 50kW scale pilot plant for researching the energy conversion of solar to renewable hydrogen production from sustainable water sources.

Title of talk: H2Xport Project – A Pilot Scale Renewable Hydrogen Plant



Dr Hieu Nguyen – Australian National University

Dr Nguyen received his PhD in photovoltaics from the Australian National University (ANU) in 2016, under the supervision of Prof Daniel Macdonald. Currently, he is a senior research fellow and senior lecturer at the ANU, leading a team of ten solar researchers. He has received several awards for excellence in teaching (2 College Dean awards) and supervision (1 College Dean and 1 university awards). Dr Nguyen's research interest spans fundamental material studies, advanced characterisation methods, and device engineering for solar PV. He has published 65 journal papers and won A\$6.8 million cash as a chief investigator (CI), including A\$2.9 million as the lead CI, from several competitive sources. Dr Nguyen's team has developed several advanced optical-based photovoltaic characterisation techniques which are being used by various research groups around the world. His team's research has been featured by many media channels worldwide.

Title of talk: The multi efforts behind solar cell efficiencies: the fundamentals, characterisation and materials engineering.



Prof. Shigeru Ikeda – Faculty of Science and Engineering, Konan University

Research works on photofunctional materials by Professor Ikeda started in 1994 when he was a master course student in Tokyo Institute of Technology (TITech). Since then he has been studying these materials and related topics for more than 20 years and published more than 100 original papers. After getting Ph. D. degree in TITech in 1999, he became an assistant professor in Hokkaido University. In 2003, he was promoted to an associate professor in Osaka University and then became a full professor in Konan University in 2016. Professor Ikeda is also an Associate Editor for Catalysis and Photocatalysis for Frontiers in Chemistry.

Title of talk: Photoelectrochemical Applications of Chalcopyrite and Kesterite Compound Thin Films



A/Prof Tom Rufford – School of Chemical Engineering, University of Queensland

Thomas (Tom) Rufford is an Associate Professor in the School of Chemical Engineering at the University of Queensland, Australia. Tom completed his Bachelor and PhD degrees in Chemical Engineering at the University of Queensland in 2000 and 2009, respectively, with four years engineering practice in the oil industry between these degrees. His research interests include electrode materials for supercapacitors and electrocatalysts for CO₂ reduction, industrial gas separation and purification technologies, and fluid–solid interactions in coal bed methane production systems. Tom has published more than 72 journal articles, 2 book chapters, and an edited book on carbon materials.

Title of talk: Controlling electrolyser flooding at high-current density in electrochemical CO₂ conversion to CO and ethylene



A/Prof. Zhenguo Huang – University of Technology Sydney

A/Professor Zhenguo Huang is leading the Hydrogen Energy Program at UTS. He was awarded a Discovery Early Career Research Award and Future Fellowships by the Australian Research Council. He is a Research Advisor appointed by the National Institute for Materials Science, Japan, a recipient of the Humboldt Research Fellowship for Experienced Researchers, the Chair of the International Hydrogen Carriers Alliance, and a graduate of Australian Institute of Company Directors. His research is centered on boron chemistry for energy conversion and storage. Research interests are in the fields of hydrogen storage materials, electrolytes, and two-dimensional boron-containing nanosheets.

Title of talk: Amine-borane systems featuring room temperature dehydrogenation



Dr Paul Feron – CSIRO Energy

Dr Paul Feron is a science leader in CSIRO Energy in Australia. He has been leading CSIRO's post-combustion capture (PCC) research since June 2007 and is currently Group Leader Sustainable Carbon Technologies. Dr Feron is a member of the Australian mirror committee for ISO TC265, which is developing standards for CO₂ capture and storage (CCS). He also is a member of the IEAGHG Executive Committee representing the Australian consortium. Previously Dr Feron worked for the Netherlands Organisation for Applied Scientific Research TNO. He has contributed extensively to the development and conduct of large multi-party, multinational CCS R&D programs in Europe, Australia and China and was a lead author for the IPCC Special Report on CCS. He co-authored more than 150 publications, is co-inventor on 16 patent applications and most recently edited the first monograph on post-combustion CO₂ capture (Absorption-Based Post-Combustion Capture of Carbon Dioxide – Woodhead Publishing). His current interests are in the realisation of concepts for added value, zero additional energy requirement CO₂-capture and Direct Air Capture.

Title of talk: Methane as renewable energy carrier



Prof. Tatsuya Kodama - Faculty of Engineering / Pacific Rim Solar Fuel System Research Center Niigata University, Japan

Prof. T. Kodama has been working in the field of concentrating solar thermochemistry (CSTC) for more than 20 years, developing the technologies on two-step water/CO₂ splitting cycles, solar coal gasification, and solar methane reforming. He has authored over 100 research papers and some international patents in CSTC field. He conducted one of the biggest Japanese CSTC R&D projects, promoted by Japan Cabinet Office in 2010-2013 (NEXT). An 100-kWth new solar beam-down system was built in Japan for demonstrating his innovative solar “particle fluidized bed” reactor to split H₂O/CO₂ to produce H₂/CO. He is currently one of the key partners of ARENA (Australian Renewable Energy Agency) project of “Solar Thermochemical Hydrogen Research and Development (2018-2022)” to demonstrate his solar particle fluidized bed reactor to split H₂O using 500 kWth solar facility of CSIRO, Newcastle, Australia.

Title of talk: Solar Thermochemical Water Splitting Cycle with a Particle Reactor



Prof Adam Lee – RMIT

Professor Lee was recently appointed Professor of Sustainable Chemistry at RMIT, having previously held a prestigious EPSRC Leadership Fellowship. He has held Chair appointments at Cardiff, Warwick, Monash, and Aston universities and is one of the world's leading mid-career researchers in heterogeneous catalysis and green chemistry, targeting the rational design of nanoengineered materials for clean catalytic technologies, and the development of spectroscopic methods for molecular insight into surface reactions. He was awarded the 2011 McBain Prize of the Society of Chemical Industry and 2012 Beilby Medal and Prize of the Royal Society of Chemistry, has published >210 peer-reviewed articles and graduated >30 PhD and MSc students. Professor Lee pioneered the application of time-resolved XPS for surface reactions, and the in situ surface analysis facility will underpin ongoing mechanistic studies into transition metal catalysed biomass valorisation, and semiconductor photocatalysts for solar fuels production and environmental depollution.

Title of talk: Hierarchically structured catalysts for sustainable energy production



Dr Tze Hao Tan – UNSW Sydney

Dr Tze Hao Tan works in the field of carbon capture and utilisation. Dr Tan spent much of his eight-year career developing techniques and materials to study C1 chemistry and light-adsorbate interactions on heterogeneous catalysts. Dr Tan graduated from the University of New South Wales, Australia, under the tutelage of Prof. Rose Amal. Following his PhD, Dr Tan joined Prof Ken Sakai's laboratory in Kyushu University, Japan, via the Japan Society for the Promotion of Science (JSPS) Fellowship. Notable works of Dr Tan are available in Nature Catalysis, Energy and Environmental Science, Nature Communications, and ACS Catalysis.

Title of talk: Pathways to light assisted CO₂ activation and potential application in solar thermal carbon capture and utilisation



Dr Gurpreet Kaur – CSIRO

Dr Gurpreet Kaur is a research scientist working in the electrochemical energy systems team in the energy technologies program of CSIRO. The major emphasis of her work is on understanding of the fundamental reaction mechanisms at the electrode / electrolyte interface and development of electrode compositions for the efficient conversion of steam / CO₂ into hydrogen / syngas. She is a key scientist responsible for the electrode development work of multidisciplinary \$2.5M ARENA project with several partners (North-western University (USA), Ben Gurion University at the Negev (Israel), Johnson Matthey (UK), ABEL Energy, Raygen Ltd) involved for further development of this technology. Dr Kaur is currently leading this project and is responsible for delivering on the final project milestone. Dr Kaur is also leading a project on electrochemical synthesis of ammonia in collaboration with RMIT and Korean Research Institute of Chemical Technology (KRICT). She has authored several technical publications including journal and conference papers. Prior to joining CSIRO, she did her PhD at Indian Institute of Technology Delhi on solid oxide fuel cells (SOFC).

Title: Solid oxide electrolyzers: Efficient technology for utilization and transportation of renewable energy in form of value-added chemicals and fuels



A/Professor Alexandr Simonov – Monash University

Dr Alexandr N. Simonov completed his PhD from the Boreskov Institute of Catalysis, Russian Federation. At present, he is a continuing academic and an ARC Future Fellow at the School of Chemistry, Monash University (Australia). Alexandr leads a *Solar Fuels* group focusing on the design and advanced characterisation of electromaterials and devices for energy conversion and storage, with a major focus on electrocatalytic synthesis and emerging photovoltaic technologies.

Title: Towards sustainable electrosynthesis of hydrogen and ammonia



Prof. Robert Willow – Macquarie University

Robert D. Willows is a professor in the Department of Molecular Sciences at Macquarie University. Robert received his PhD in Biochemistry from UNSW in 1992. He then worked at Carlsberg Laboratory (1992-1995) and Brown University (1996-1997) on enzymes involved in the biosynthesis of bacteriochlorophyll, chlorophylls and bilins. His research career has concentrated on the biochemical and structural characterisation of complex enzyme systems, primarily those involved in tetrapyrrole synthesis in photosynthetic organisms. He was co-discoverer of chlorophyll f from a novel cyanobacteria isolated from stromatolites. He has been a leader in promoting and teaching Synthetic Biology at undergraduate level through developing curriculum and mentoring iGEM teams at Macquarie University since 2010. He is currently utilizing synthetic biology techniques in developing and optimising biohydrogen production in bacteria.

Title: Optimising biohydrogen production in bacteria using synthetic biology



Prof. Gerry Swiegers – University of Wollongong

Gerhard (Gerry) F. Swiegers is a Professor at the University of Wollongong, Australia. He leads an active research program focusing on electrochemical catalysis and the production of hydrogen from water using renewable electricity. He also works in the fields of electrocatalytic process engineering and industrial electrochemistry. He has founded 7 spin-off companies and licensed out 3 new technologies in the last 20 years that have attracted an estimated \$100 million in private investment. He has published 2 books, 135 scientific contributions, and 52 patent families. His inventions have found use in the pharmaceutical, apparel, casino chip, agricultural, automobile, energy and other industries.

Title of talk: A New Class of Bubble-Free Water Electrolyzer that is Highly Energy Efficient



Dr Nick Burke – Carbon Innovation, Victoria Dept. of Jobs, Precincts and Regions

Dr Nick Burke is Manager Carbon Innovation with the Victorian Department of Jobs, Precincts and Regions. In this role he engages with a range of stakeholders to provide guidance and facilitation support that enables the progression of industries based on carbon technologies in Australia. Prior to this role he worked at CSIRO as a research scientist in the Energy business unit, mainly in the areas of natural gas processing and conversion. He has a bachelor's degree in Industrial Chemistry and a PhD in Chemical Engineering from UNSW.

Title: What part can coal-derived hydrogen play in Australia's Energy Future?



A/Prof Yun Hau Ng – CARE Lab, City University of Hong Kong

Presently an Associate Professor in the School of Energy and Environment at City University of Hong Kong. APEC ASPIRE Prize recipient for collective efforts in artificial photosynthesis research for clean hydrogen production. His work in water splitting was recognised with the award of Honda-Fujishima Prize. Previously a senior lecturer in the School of Chemical Engineering, The University of New South Wales (UNSW), Sydney, Australia. Ng joined the ARC Centre of Excellence for Functional Nanomaterials, Particles and Catalysis Research Group (PARTCAT), Sch. Chem Eng. UNSW as a postdoctoral researcher in April 2009 to initiate a research on hybrid inorganic-organic nanostructures for solar energy conversion. He held the fellowship of APD from the Australian Research Council. Currently a Chartered Chemist of the Royal Australian Chemical Institute (RACI).

Title of talk: Solar Fuels from Photocatalysis



Prof John Andrews – RMIT

Professor Andrews is an expert in sustainable energy, specialising in hydrogen energy storage to ensure continuous and reliable supply from intermittent renewable energy. He is currently leading an ARENA-funded project into 'A proton flow reactor system for medium- and large-scale electrical energy storage and bulk export of hydrogenated carbon-based material'. This ~\$1 m project started in August 2018 and is due to be completed in August 2021. Eldor Corporation in Italy is an industry partner, and Kyushu University and the Institute for Carbon Neutral Energy Research in Japan are academic research partners. Professor John Andrews' book *Living Better with Less* (Penguin 1981) was one of the first works to propose sustainable development for Australia. He played a pioneering role in assessing the potential and encouraging utilisation of wind energy for electricity generation in Australia. His current research interests are in renewable-energy – hydrogen systems for stationary and vehicular applications. His publications include two books, four invited review chapters, 50 journal and conference papers, 18 major reports, 14 articles, and the proceedings of a major scientific conference (lead editor). He was the founder of RMIT's successful Master of Engineering (Sustainable Energy) program.

Title of talk: A proton flow reactor system for electrical energy storage and bulk export of hydrogen as hydrogenated carbon-based material



Prof Michelle Spencer - RMIT

Professor Spencer's research specialises in computational chemistry. She focuses on using density functional theory and ab initio molecular dynamics simulations to determine the structure, dynamic properties and surface reactions of materials and nanomaterials for applications in electronic devices, gas sensors and batteries.

She collaborates with industry and local and international researchers and has secured research grants from both industry and government. She collaborates extensively with Defence Science and Technology (DST) and the CSIRO. She is also an Associate Investigator in the ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET). Professor Spencer is passionate about digital innovations in science education, and has developed a mobile application, called Chirality-2, for teaching concepts in undergraduate chemistry. The app is available to download for free on the Google Play and Apple stores.

Title of talk: Reaction mechanism of proton storage in a proton flow reactor system: insights from DFT calculations



Jorge Martin Gistau – Ricardo Rail Australia Pty Ltd.

Jorge is a versatile Project-Manager, who has embraced and championed innovation to deliver projects within the Rail Industry to positively impact society.

Having worked successfully in both the public and private sectors in Australia, Spain, England and Germany, Jorge has extensive experience executing and managing international rolling stock projects. Developing his extensive skillset through his experience as an industrial Engineer, Project Manager and Supply Chain Manager, Jorge delivers innovative and effective engineering solutions. Most recently, Jorge has managed multiple aspects of the Regional Rail Project, which will deliver a new regional fleet for Transport for NSW.

Jorge is an active promoter of innovation and he will present on Hydrogen Transport Solutions where Ricardo plc has played a key role. Ricardo plc has placed decarbonisation and sustainability at the heart of its strategy. Ricardo plc has an extensive range of skills relating to the hydrogen agenda, from policy development to infrastructure feasibility through to implementation and integration of hydrogen-based technologies for global transport applications.

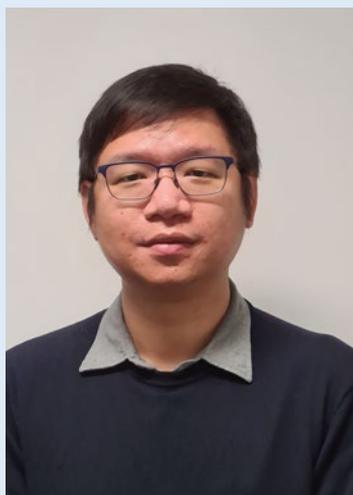
Title of talk: Delivering Hydrogen Transport Solutions Fit for the Future



Dr Emanuelle Frery – CSIRO

Emanuelle Frery is a CSIRO senior research scientist known for her recent discovery of Natural Hydrogen seeps in Australia. She loves to lead multi-discipline science projects and apply her expertise in structural geology to comprehensive assessments of energy production impact on the groundwater systems and the environment. She is passionate about fluid and gas circulation along natural faults and the impact of those circulations on the seismic cycle. She acquired a worldwide academic expertise in this field with a PhD thesis on the circulation recorded in the well-known red sandstone of the Colorado Plateau and her implication in the IODP research. Before joining CSIRO, she also worked in the oil and gas industry as a seismic interpreter and a petroleum system analyst.

Title of talk: Natural Hydrogen Seeps – Implications for Underground Storage



Dr Xunyu Lu - UNSW Sydney

Xunyu Lu is currently a Scientia Senior Lecturer at the School of Chemical Engineering, University of New South Wales (UNSW). He obtained his Ph.D. degree at UNSW in 2014. His research is mainly focused on the rational design and preparation of cost-effective and active catalysts for electrochemical energy conversion reactions, design and fabrication of energy devices based on the novel catalyst materials, and integration of the energy devices with state-of-the-art photovoltaic cells to realize the production of renewable chemicals and fuels with high energy conversion efficiency, high selectivity, and low cost.

Title of talk: Efficient Solar-to-Hydrogen Conversion Process enabled by Photovoltaic Electrolysis



Dr Zhaojun Han – UNSW Sydney / CSIRO

Dr. Zhaojun Han is currently a Senior Lecturer at UNSW and a Senior Research Scientist at CSIRO. He graduated with PhD and B.Eng both from Electrical and Electronic Engineering, Nanyang Technological University, Singapore. His research focuses on developing low-dimensional functional materials to tackle the challenges in materials, energy and environmental science. He has published 1 technical report, 2 book chapters, 4 patents, and 120 peer-reviewed journal papers. The total citations of his publications are ~4,500 and H-index is 36. He is the key inventor of two graphene-based technologies, the GraphAir technology and the vertical branched graphene technology, which have been/are undergoing commercialisation. He is the recipient of 40 under 40 Most Influential Asian-Australian, CSIRO Corporate Citizen Award, Australia-China Young Scientists Exchange Program Award, ATSE Priming Grant Award, Julius Career Award, and DECRA (2013-2016). He is also a CI in ARC Research Hub for Connected Sensors for Health.

Title of talk: 2D Materials-based Hybrid Electrocatalysts for Hydrogen Generation



Dr Qiyuan Li – UNSW Sydney

Dr. Qiyuan Li is a postdoctoral research associate from the School of Chemical Engineering, The University of New South Wales (UNSW). He has received a Ph.D. degree from the school of mechanical engineering, UNSW in 2016.

His research focused on developing new modules/systems for solar energy collection, water treatment and hydrogen production. Currently, he is working on a project 'A Zero-Emission Tandem Array for Transforming Waste Biomass into Renewable Hydrogen'.

Title of talk: Development of A PV/Thermal Solar Collector for Transforming Waste Sugar to Hydrogen.

INDUSTRY SPEAKERS PROFILE



Dr Alan Finkel – Special Adviser to the Australian Government on Low Emissions Technology

Dr Finkel is a neuroscientist, engineer and entrepreneur. He served as Australia’s Chief Scientist from 2016 to 2020. Dr Finkel led the development of the Technology Investment Roadmap: First Low Emissions Technology Statement 2020; Australia’s National Hydrogen Strategy (2019); Review into the National Electricity Market (“Finkel Review”) (2017). Dr Finkel also led the Expert Advisory Panel for the CSIRO Report on Climate and Disaster Resilience (2020), STEM Industry Partnership Forum report (2018), National Research Infrastructure Roadmap (2016). At the request of National Cabinet, he led a systems and operations review in all states and territories to enable efficient COVID-19 testing, contact tracing, outbreak management and exchange of case and outbreak data. Dr Finkel is also Chair of Stile Education, and Chair of the Australian Government’s Technology Investment Advisory Council.

Title of the Talk: Unlocking Australia’s Hydrogen Economy



Mr John O’Brien – Senior Partner, Financial Advisory, Deloitte

John O’Brien joined Deloitte Australia in 2018 as a Financial Advisory partner. With more than 20 years of experience in the Australian and Asian clean energy and clean technology sectors, he provides strategic guidance to government, private sector operators, and large energy consumers and investors on issues around decarbonization, energy transition, and environmental technologies. His key expertise includes technology assessment, project development, project financing, risk and opportunity assessment, commercial and financial analysis, policy advice, and strategic growth strategies. In 2007, O’Brien established Australian CleanTech, a corporate advisory firm focused on environmental technologies, which he ran until joining Deloitte in 2018. He has also published two books on the opportunities emerging from the transition to a low-carbon economy. O’Brien has engineering degrees from Oxford University and Trinity College, Dublin, and holds an MBA from Adelaide University.

Title of talk: The role of hydrogen in achieving net zero at the least possible cost for the economy



Professor Peta Ashworth OAM – Academy Director of the Andrew N.Liveris Academy for Innovation and Leadership, Chair in Sustainable Energy Futures, Univ of Queensland.

Peta brings over thirty years of experience working in a range of senior management and research roles. Peta established and led the Science into Society Group (SISG) within CSIRO's Division of Earth Science and Resource Engineering. The Group specialised in interdisciplinary research at the interface between science and society and applied social science expertise to understand human responses to nationally-identified challenges. Peta's main research interest is how to deliver information to best effect and facilitating dialogue across a broad range of stakeholders around complex and contested issues.

Title of talk: Hydrogen Industry and the Public

Unanticipated problems in H₂ Economy Session



Dr. Bart Kolodziejczyk – Chief Scientist, Fortescue Metal Group

Bart Kolodziejczyk has been working in the hydrogen and renewables space for over a decade. He has advised the UN, NATO, G20, OECD, and European Commission on science, technology, innovation, and policy and was named one of MIT Technology Review's Innovators Under 35 for his conductive polymers, which reduce the cost of solar panels and are applied in medicine and bio-sensing. Dr. Kolodziejczyk was featured as one of 100 Visionary Leaders by Real Leaders Magazine. Bart has appeared in numerous publications, including Forbes Magazine, Business Insider, as well as many newspapers and radio stations in the US, Australia, Poland and abroad. Kolodziejczyk is an active Member of the Global Young Academy and IUCN, Fellow of the Royal Society of Arts and Fellow of the Linnean Society of London, Fellow International of the Explorers Club and is a Chartered Environmentalist. Kolodziejczyk holds five master degree's and two PhDs covering fields from mechanical engineering, through renewable energy science and microelectronics to European studies. In his free time, Kolodziejczyk enjoys traveling and scuba diving.

Title: Transitioning from Fossil Fuels to Hydrogen



Mr Tim Stock – Project Director, Hydrogen and Clean Energy, NSW Department of Planning, Industry and Environment

Tim has over 15 years commercial and government experience in the clean energy industry in Australia and abroad. Currently he is the Project Director Hydrogen and Clean energy programs at the NSW department of Planning, Industry Environment where he is leading the development of a NSW Hydrogen Strategy and responsible for the delivery of the \$70m hydrogen hubs program. In addition, Tim leads a number of other governments led sustainable and renewable energy initiatives, around demand response and distributed energy resources and is also the chair of the National GreenPower Accreditation program.

Title: NSW Hydrogen Strategy – pathway to a NSW Hydrogen economy.



Ms Anne Foster – Director, Quinbrook Infrastructure

Anne Foster is a specialist renewable energy, energy transformation and ESG Private Equity & Venture Capital investor and Global Head of ESG at Quinbrook Infrastructure Partners. She has invested or advised on over US\$3bn globally in energy and infrastructure projects and has worked on some of the world's largest solar and storage projects and in emerging technologies that are central to enabling our future energy distribution and grids. She has advised companies including Fortescue, BHP Billiton, Woodside Petroleum and Shell.

Title of talk: Renewables/hydrogen project financing and impact on future hydrogen projects



Ms Simone O'Sullivan – Director Energy Growth – Energy Estate

Simone's professional career has centred around climate change solutions, renewable energy and utilities from consulting firms such as PwC to government agencies and large utility companies. She has a track record in helping forecast, position and develop new business models, with a strong focus on partnerships and collaboration. Before joining Energy Estate, she lived in Canada and the US for 10 years where she completed a Masters of Sustainable Management at Columbia University and ran her own sustainability consulting business. Previous to that, she built and ran a renewable energy fund for Sustainability Victoria, developed climate change policy for Origin Energy and was involved in a start up in biofuels in Vietnam and Thailand.

Title: Reindustrialising the Hunter - Hunter Hydrogen Network



Mr Andrew Dickson – Development Manager, Green Hydrogen & Ammonia Project, CWP Global

Andrew Dickson is Development Manager with CWP Global, which has a portfolio of export-oriented green hydrogen & ammonia projects in Australia (including the 26GW Asian Renewable Energy Hub project (www.asianrehub.com) and the recently announced 50GW Western Green Energy Hub), in Africa and in South America. He has been a renewable energy project developer since 2004 and has developed wind / solar PV / solar thermal / microgrids / hydrogen / ammonia projects in most Australian states. He has a Bachelor of Electrical and Electronic Engineering degree from the University of New South Wales and a Master of Science and Technology commercialisation degree from the University of Adelaide.

Title: Renewable Energy at Oil and Gas Scale



Dr Matthew Brannock – Technical Director, GHD

Matthew Brannock has over 20 years of experience covering computational modelling of water treatment processes and the design of demineralisation, desalination and brine management processes within both engineering consulting and academia. This work has resulted in more than 30 journal and conference papers. He's worked on projects ranging from the feasibility and pilot testing to detailed design in the municipal, resource and energy sectors. He is also the co-creator of the water and wastewater treatment design & simulation software platform EVS:Water. Over the last 2 years Matthew has worked on the design of water treatment processes for several varied hydrogen projects for which he'll pass on his experiences of today.

Title of talk: Challenges and opportunities for treatment of water for hydrogen production

Unanticipated problems in H₂ Project Development Session



Mr Alex Trajkov – Executive Manager, Trading & Logistics, H2U Pty Ltd.

Alex is a top-performing, strategic-thinking professional with over 18 years' experience in chemicals business management (in particular Ammonia and Bulk Gases). Self-motivated with experience managing multiple projects simultaneously. Extensive expertise in managing multifaceted commercial projects; global RFT, ranging from commodity chemicals trading, product and/or market development to large mining developments. Highly skilled in needs assessment, quality assurance, managing supply chains.

Title: Experience in scaling up Renewable Ammonia Plants



Mr Michael van Baarle – CEO, ABEL Energy (Tasmania)

Michael is a co-founder and CEO of ABEL Energy. Michael has been involved in developing projects for synthetic fuel production since 2006 following a 20-year legal career. As well as leading ABEL Energy, Michael is directly responsible for legal, corporate and public affairs for the company and the first project. He has developed a broad knowledge of the production and use of methanol and DME as fuels, and also has a long history of engagement with decision-makers at all levels of government in Australia and the USA.

Title: Challenges for people to accept low carbon carrier, financing



Mr Daniel Krosch – Mechanical Engineer, GPA Engineering

Daniel is a Mechanical Engineer at GPA Engineering and holds a master's from QUT. He has a experience in renewable energy projects, which spans the entire development lifecycle from initiation to first start-up. He has delivered projects in hydrogen supply chains from mobility to export. This is underpinned by his fundamental understanding of fuel cells, electrolyzers and other emerging technology. Daniel is an advisor to the Future Fuels Cooperative Research Centre, sitting on the research steering committee. He is also a member of ME-03 Hydrogen Australian Standards and a part of the specialist team tasked with drafting the new "The storage and handling of hydrogen" standard. Daniel also sits on the International Hydrogen Safety (HySafe) scientific committee. Currently, Daniel is focusing on the steps required to enable a hydrogen in Australia. A key focus area is development and optimisation of energy hubs.

Title: Challenges in Designing Hydrogen Systems



Mr Timothy Meyers – Sales Manager for Asia Pacific, MAN Energy Solutions

Timothy Meyers is the Head of Power Sales for MAN Energy Solutions in the Australian and Pacific markets. He has been in sales and business development at MAN for ten years and lived in Germany from 2008 to 2018. Prior to moving back to Australia, he was responsible for the sales and business development of power plants in the Caribbean for MAN. He has been involved in power projects in Europe, the Americas, the Middle East and Asia. On top of power generation projects, Tim is passionate and active in developing a hydrogen industry in Australia both for domestic use and for export.

Title: How can we use Hydrogen to iteratively decarbonise



Mr Greg Bowyer – Manager, Western Sydney, Principal, GHD Senior Technical Director / Infrastructure Project Director

Greg Bowyer is the Manager, Western Sydney, Senior Technical Director/ Infrastructure Project Director at GHD. He is currently driving GHD's Western Sydney community and growth, looking to integrate innovative architectural and engineering thinking, property owners, investment options, thought leadership and alternate client futures to build new and lasting communities in Western Sydney. As a civil engineering and company director qualified executive he has over 25 years' experience, most recently being responsible for a team of over 100 professionals delivering a full range of engineering services, \$200m+ capital construction projects and client relationship development and management.

Title of talk: Commercialisation and integration challenges of new hydrogen technologies



H.E. Phillip Green OAM – Australian Ambassador to Germany, DFAT

Philip Green is the Australian Ambassador to Germany, Switzerland and Liechtenstein. Mr Green is a senior career officer with the Department of Foreign Affairs and Trade and was most recently First Assistant Secretary, United States and Indo-Pacific Strategy Division. He has previously served overseas as Head of Mission in Singapore, South Africa and Kenya. He has served previously as Ambassador and/or High Commissioner in Singapore (2012-2016), South Africa (2004-2008), and Kenya (1998-2000). In his last assignment in Canberra (2018-2019), Mr Green was responsible for leading Australia’s Indo-Pacific Strategy as well as relations with the United States, Canada and ASEAN. Earlier, Mr Green served as International Adviser to Australian Prime Minister Kevin Rudd (2009-2010) and as Chief of Staff when Mr Rudd was Foreign Minister (2010-2012). He led the Secretariat for the Review of Australian Intelligence Agencies in 2004. Mr Green was awarded the Order of Australia Medal in 2003 for his role in the response to the Bali terrorist tragedy. He holds a Bachelor of Arts with First Class Honours and a Bachelor of Laws from the University of Sydney. He has been awarded honorary degrees from the James Cook University and Murdoch University.



H.E. Dr Thomas Fitschen – German Ambassador to Australia, Foreign Office

Dr Thomas Fitschen joined the German Foreign Service in 1990.

Since 7 August 2019 he is the German Ambassador to Australia. Before coming to Canberra he was the Federal Foreign Office’s Special Representative for Cyber Foreign Policy and Cybersecurity. In addition to a number of positions at Headquarters he served abroad as Deputy Permanent Representative of Germany to the United Nations in Geneva, as the legal advisor and deputy head of the political section of the German UN Mission in New York, as head of the consular section at the Embassy of Germany in the Philippines and as desk officer for human right and social issues at the German UN Mission in New York. Ambassador Fitschen is a lawyer by training (University of Kiel, Germany) and holds a doctorate in international law from the University of Saarbrücken. He holds memberships in the German Society of International Law (DGIR), the European Society of International Law (ESIL) and the German United Nations Association (DGVN).



Prof Dr Robert Schlögl – Director, Fritz-Haber-Institut der Max-Planck-Gesellschaft

Dr Robert Schlögl completed his study of chemistry from Munich Univ. and obtained the doctorate from Munich Univ. (1982). He was a postdoctoral fellow in Cambridge and Basel, and at the Fritz Haber Institute of the Max Planck Society and "Habilitation" in chemistry at the Technical University Berlin (1989). He joined Frankfurt/Main Univ in 1989 as a Professor of Inorganic Chemistry (C4 level) and became the Univ. (1989-1994), and became the Director and Scientific Member at the Fritz-Haber-Institut of the Max Planck Society in 1994. Prof Schlögl is also an Honorary Professor of Chemistry at Technical University Berlin since 1994 and an Honorary Professor of Chemistry at the Humboldt University Berlin since 1999. He is a chemist and catalysis researcher. His research focuses on heterogeneous catalysis and materials for energy storage concepts. With his work, he has contributed to a new understanding of catalytically active materials. More recently, he has been working on energy systems of the future and the complex challenges of the energy revolution.



Mr Holger Lösch – Deputy Director General, BDI e.V.

From 1983 to 1992 he studied Political Sciences, History and German at the Ludwig Maximilians University in Munich. Even during his studies he worked as a journalist and editor in the television section of Bayerischer Rundfunk. From 1995 he was head of the staff of the television directorate at Bayerischer Rundfunk, subsequently moving on to assume the management of Central Programme Coordination in 1998. In 2001 Holger Lösch moved from the Bayerischer Rundfunk to the Schörghuber Group in Munich and was head of the central area Communication and Marketing until 2007. From 2006 he was also a member of the corporate management. From 2007 to 2008 he was in charge of the management of Corporate Development, Communications and Customer Relation Management of Arabella Hotel Holding Munich. In 2008 he was appointed head of Communications and Marketing at the Federation of German Industries (BDI), also becoming a member of the management in 2009. Holger Lösch has been a member of the BDI Executive Board since July 2011 and Deputy Director General of the BDI since April 2017.



A/Prof Ian MacGill – Joint Director, Centre for Energy and Environmental Market (CEEM) at UNSW Sydney.

Dr Iain MacGill is an Associate Professor in the School of Electrical Engineering and Telecommunications at the University of New South Wales, and Joint Director (Engineering) for the University’s Centre for Energy and Environmental Markets (CEEM). He leads work in two of CEEM’s three research areas - Sustainable Energy Transformation including energy technology assessment and renewable energy integration, and Distributed energy systems including ‘smart grids’ and ‘smart’ homes, distributed generation and demand-side participation. He also has research interests in energy and climate policy. He has run industry short courses and consulted to industry and government clients in these areas here in Australia and internationally. He is the Responsible Australian Expert on the International Energy Agency’s PV Power Systems Task 14 on high PV penetrations in the electricity grid and an invited expert for the technical reference groups of the Federal Government’s Australian Energy Technology Assessment, the Australian Energy Market Operator’s future energy scenarios planning process and, previously, the Australian Energy Market Commission’s Demand-Side Participation Review. Iain has a PhD (Electrical Engineering) from UNSW, and a M.Eng.Sc. (Biomedical) and B.E. from the University of Melbourne. Former roles include ‘smart control systems’ consulting in the Australian Mining and Mineral Processing industry, and several years in Washington DC as a senior policy analyst in the environmental NGO sector. CEEM itself undertakes interdisciplinary research in the analysis and design of energy and environmental markets and their associated policy frameworks. It brings together researchers from five UNSW Faculties with project funding from partners including the Australian Federal Government, CSIRO, State Governments and industry.



Dr Will Rayward Smith – Partner, Financial Advisory, Deloitte

Will is a specialist in decarbonisation and the clean energy transition. He is driven to accelerate the transformation to the low-carbon world and to support his clients successfully navigate the risks and unlock the significant opportunities. Will joined Deloitte in 2019 with hands-on experience of growing a low-carbon business, having founded SunSHIFT, a provider of solar power to the mining sector. As General Manager, Will scaled SunSHIFT within three years into a profitable business, owned by the global engineering and construction company Laing O’Rourke. Achievements at SunSHIFT include three grants awarded by the Federal Government totalling AUD 3 million, the delivery of Australia’s first integration of solar with an off-grid gas power plant and completion of the 89MW Clermont and 110 MW Wemen solar farms. Will has a PhD in Mathematics from the University of Cambridge and has previously worked for Arup, the UK Government’s Department of Energy and Climate Change (DECC) and Azuri Technologies.



Dr Rahman Daiyan – Lecturer and Chief Investigator ARC Training Centre for Global Hydrogen Economy (GlobH2E), UNSW Sydney

Dr Rahman Daiyan is a Lecturer at the School of Chemical Engineering at The University of New South Wales. His research direction is to explore artificial photosynthesis through the development of inexpensive and scalable nanomaterials and high throughput systems to tackle climate change (Carbon dioxide reduction) as well as to promote alternate fuels (hydrogen production). Daiyan is also the Chief Investigator for the ARC Training Centre for the Global Hydrogen Economy, NSW Power-to-X and DFAT HySupply Project.

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EF4 2021 Conference Program

Start	Day 1	
9:00	Welcome and Opening speech - Mr Grant King (UNSW & Climate Change Authority)	
9.15	PT1: Artificial photosynthesis using powdered photocatalyst materials - Prof. Akihiko Kudo (Tokyo Univ of Science) Chair: Prof Rose Amal	
9.55	Plenary Q&A	
10:00	Morning Tea	
	Sessions (H2 Generation) - Chair: A/Prof Jason Scott	Sessions (H2 Carriers) - Chair: Dr Tze Hao Tan
10.30	KT1: High efficiency direct solar hydrogen generation - Prof Kylie Catchpole (ANU)	KT2: Towards Solar Fuels - Hydrogen and Ammonia - Prof Doug Macfarlane (Monash Univ)
11:00	IT1: Solar Thermochemical Water Splitting Cycle with a Particle Reactor - Prof Tatsuya Kodama (Niigata Univ., Japan)	IT5: Process considerations for electrochemically driven green ammonia and carbon negative materials - Dr Jessica Allen (Univ of Newcastle)
11:20	IT2: Advanced Semiconductor and Catalytic Materials for Direct Solar Hydrogen Generation - Dr Siva Karuturi (ANU)	IT6: Amine-borane systems featuring room temperature dehydrogenation - A/Prof Zhenguang Huang (UTS)
11:40	IT3: Photoelectrochemical Applications of Chalcopyrite and Kesterite Compound Thin Films - Dr Shigeru Ikeda (Konan Univ, Japan)	IT7: Methane as renewable energy carrier - Dr Paul Feron (CSIRO)
12:00	IT4: Photocatalysts for H2 Production Based on Metal Clusters as Co-Catalysts - Prof Gunther Andersson (Flinders Univ)	NT4 Efficient Solar-to-Hydrogen Conversion Process enabled by Photovoltaic Electrolysis - Dr Xunyu Lu (UNSW)
12:20	IT15: Solid oxide electrolyzers: Efficient technology for utilization and transportation of renewable energy in form of value-added chemicals and fuels - Dr Gupreet Kaur (CSIRO)	
12:40	Lunch	
	Sessions (H2 Carriers) - Chair: Prof Chuan Zhao	Sessions (H2 Storage) - Chair: Prof Francois Aguey Zinsou
13:40	KT3: Towards sustainable electrosynthesis of hydrogen and ammonia - A/Prof Alexandr Simonov (Monash Univ)	KT4: Is there a role for metal-hydride hydrogen storage in the developing hydrogen economy? - Prof Evan Gray (Griffith Univ)
14:10	IT9: Hierarchically structured catalysts for sustainable energy production - Prof Adam Lee (RMIT)	NT3: Options for Underground Storage of Hydrogen in Australia - Dr Jonathan Ennis-King (CSIRO)
14:30	IT10: Controlling electrolyser flooding at high-current density in electrochemical CO2 conversion to CO and ethylene - Dr Thomas Rufford (Univ of Queensland)	IT12: MBNH materials for solid-state hydrogen storage – Focus on alkali and alkaline-earth hydrazinidoboranes - Prof Umit Demirci (Univ of Montpellier, France)
14:50	IT22: Heterogeneous Molecular Electrocatalysts for Carbon Dioxide Reduction in Water - Dr Yijiao Jiang (Macquarie Univ)	KT5: Hydrogen Generation and Storage: from Materials to Components - Prof Thomas Klassen (Helmholtz-Zentrum Geesthacht)
15:10	IT11: Pathways to light assisted CO2 activation and potential application in solar thermal carbon capture and utilisation - Dr Tze Hao Tan (UNSW)	
15:30	Afternoon Tea	
16:00	PT2: A personal perspective into the catalysts for hydrogen production - Prof Paolo Fornasiero (Univ of Trieste, Italy) - Chair: Dr Emma Lovell	
16:40	Plenary Q&A	
16:45	Poster Session and Virtual Networking (via Wonder.me)	

DAY 2	
9:00	Welcome + House Keeping
9:05	PT3: Sunlight-Driven Hydrogen Formation by Membrane-Supported Photoelectrochemical Water Splitting - Prof Nathan Lewis (Caltech) Chair: A/Prof Jason Scott
9:45	Plenary Q&A
9:50	Morning tea
10:30	PT4: By passing wires - Monolithic Integrated Devices for Solar Driven Hydrogen Production and Solar Batteries - Prof Anita Ho-Baillie (Sydney University) Chair: Prof Lianzhou Wang
11:10	Plenary Q&A
	Sessions (H2 Generation) - Chair: Dr Xunyu Lu
	Sessions (H2 Applications) Chair: Dr Alex Simonov
11:15	KT6: Solar Fuels from Photocatalysis - A/Prof Yunhau Ng (City University of Hongkong)
	KT7: Emerging roles for hydrogen in decarbonizing heavy industrial processes - Prof Gus Nathan (Univ of Adelaide)
11:45	IT13: A New Class of Bubble Free Water Electrolyzer that is Highly Energy Efficient - Prof Gerry Sweigers (Univ of Wollongong)
	IT17: H2Xport Project – A Pilot Scale Renewable Hydrogen Plant - A/Prof Jonathan Love (QUT)
12:05	IT14: Optimising Biohydrogen Production in Bacteria using Synthetic Biology - Prof Robert Willows (Macquarie Univ)
	IT20: A proton flow reactor system for electrical energy storage and bulk export of hydrogen as hydrogenated carbon-based material - Prof John Andrews (RMIT)
12:25	IT16: Understanding Hydrogen Autoignition and Knocking in Spark-Ignition IC Engines - Dr Farzad Poursadegh (Melbourne Energy Institute)
	IT21: Reaction mechanism of proton storage in a proton flow reactor system: insights from DFT calculations - Prof Michelle Spencer (RMIT)
12:45	NT1: 2D materials-based hybrid electrocatalysts for hydrogen generation - Dr Zhaojun Han (UNSW)
	NT6 Natural hydrogen seeps – implications for underground storage - Dr Ema Frery (CSIRO)
13:05	Lunch
	Sessions (Green e) Chair: A/Prof Yunhau Ng
	Sessions (H2 transitions) - Chair:Dr Kathy Witt
14:05	KT9: Hybrid Perovskite Quantum Dots for High Efficiency Solar Cells - Prof Lianzhou Wang (Univ of Queensland)
	KT10: What part can coal-derived hydrogen play in Victoria's Energy Future? - Dr Nick Burke (Department of Jobs, Precincts and Regions, Victoria govt)
14:35	IT18: The multi efforts behind solar cell efficiencies: the fundamentals, characterisation and materials engineering - Dr Hieu Nguyen (ANU)
	NT2 Hydrogen Industry Progress Indicators: A Data Framework for tracking the Hydrogen Value Chain - Dr Lavinia Poruschi (CSIRO)
14:55	IT19: Design of Green Kesterite for Solar Photovoltaic and Photoelectrochemical CO2 reduction - A/Prof Xiaojing Hao (UNSW)
	NT7 Delivering Hydrogen Transport Solutions Fit for the Future - Mr Jorge Martin Gistau (Ricardo Plc)
15:15	NT8 Development of A PV/Thermal Solar Collector for Transforming Waste Sugar to Hydrogen - Dr Qiyuan Li (UNSW)
	NT5 Public Perceptions Towards Hydrogen Energy Technologies Across the Value Chain - Dr Mitchell Scovell (CSIRO)
15:35	Afternoon tea
16:00	PT5: FeTi-based intermetallic compounds for large-scale stationary hydrogen storage - Dr Fermin Cuevas (CNRS, France) Chair: Prof Francois Aguey Zinsou
16:40	Plenary Q&A
16:45	Poster Award presentation

DAY 3	
9:00	Welcome to Day 3 - Prof Rose Amal
9:10	Unlocking Australia's hydrogen economy - Dr Alan Finkel - 20 min
9:30	The role of hydrogen in achieving net zero at the least possible cost for the economy - Mr. John O'Brien (Deloitte) ~ 20min
9:50	Hydrogen industry and the public - Prof Peta Ashworth (UQ) ~ 20min
10:10	Plenary Q&A (15 min) - Moderator: Ms Justine Jarvinen
10:25	Morning Tea (15min)
10:40	Unanticipated problems in H₂ Economy - Chair:A/Prof Iain Macgill ~ 5min
10:45	Transitioning from Fossil-Fuels to Hydrogen - Dr. Bart Kolodziejczyk (Fortescue Metal Group) ~15min
11:00	NSW Hydrogen Strategy – pathway to a NSW Hydrogen economy - Mr Tim Stock (NSW Dept of Planning, Industry and Environment) ~ 15min
11:15	Financing Green Hydrogen: Global Demand for ESG-Focused Green Hydrogen Solutions - Ms Anne Foster (Quinbrook Infrastructure) ~ 15min
11:30	Reindustrialising the Hunter - Hunter Hydrogen Network - Ms Simone O'Sullivan (Energy Estate) ~ 15min
11:45	Renewable Energy at Oil and Gas Scale - Mr Andrew Dickson (CWP Global) ~ 15min
12:00	Challenges and opportunities for treatment of water for hydrogen production- Dr. Matthew Brannock (GHD) - 15 min
12:15	Panel Discussion on Requirement for Hydrogen Enabling Policies: 30 min
12:45	Lunch ~ 1hr
14:00	Unanticipated problems in Hydrogen Project Development - Chair: Prof Greg Leslie ~ 5min
14:05	Experience in scaling up Renewable Ammonia Plants - Mr Alex Trajkov (H2Utility)
14:20	Challenges for people to accept low carbon carrier, financing - Mr Michael van Baarle (ABEL Energy)
14:35	Challenges in Designing Hydrogen Systems - Mr Daniel Krosch (GPA Engineering)
14:50	How can we use Hydrogen to iteratively decarbonise - Mr Timothy Meyers (MAN Energy Solutions)
15:05	Commercialisation and integration challenges of new hydrogen technologies- Mr Greg Bowyer (GHD)
15:20	Panel Discussion ~25 min
15:45	Afternoon tea ~ 15 min
16:00	Exploring Opportunities for renewable H₂ export from Australia to Germany- HySupply (Ambassador Philip Green OAM, Ambassador Dr Thomas Fitschen, Prof Robert Schloghl, Mr Holger Losch and Dr Will Rayward Smith - Chair & Moderator: Prof Sami Kara, Dr Rahman Daiyan/Prof Iain MacGill
17:30	Closing Remarks - Prof Francois Aguey Zinsou

Artificial photosynthesis using powdered photocatalyst materials

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Photocatalytic water splitting and CO₂ reduction are promising reactions to solve resources, energy, and environment issues. These reactions are regarded as artificial photosynthesis, because light energy is converted to storable chemical energy. Photocatalyst systems based on powder materials will be economical because of the simplicity. In the present paper, I introduce various metal oxide and sulfide photocatalysts and semiconductor photoelectrodes for water splitting and CO₂ reduction.

Rh_{0.5}Cr_{1.5}O₃/AgTaO₃ (BG: 3.4 eV) of a valence-band-controlled metal oxide photocatalyst shows an excellent activity for water splitting [1]. The photocatalyst gives 40% of an apparent quantum yield at 340 nm and 0.13% of STH (solar to H₂ energy conversion efficiency). Rh and Sb-codoped SrTiO₃ photocatalyst (EG: 2.3 eV) loaded with IrO₂ is active for water splitting under visible light as a single particle-type photocatalyst [2]. SrTiO₃:Rh of a H₂-evolving photocatalyst and BiVO₄ of an O₂-evolving photocatalyst can be employed for various type of Z-schematic photocatalyst systems with Fe³⁺/Fe²⁺, [Co(bpy)₃]^{3+/2+}, [Co(phen)₃]^{3+/2+} and RGO as an electron mediator, and even without an electron mediator [3]. Ag cocatalyst-loaded ALa₄Ti₄O₁₅ (A = Ca, Sr, and Ba) [4] and NaTaO₃:Ba photocatalysts [5] show high activities and selectivities for CO₂ reduction to form CO in an aqueous medium. Z-scheme systems working under visible light irradiation for CO₂ reduction using water as an electron donor can be constructed with metal sulfide photocatalysts of a CO₂-reducing photocatalyst with BiVO₄ of an O₂-evolving photocatalyst [6].

References

- [1] *Chem. Sci.*, 11, 2330 (2020).
- [2] *Chem. Commun.* 50, 2543 (2014).
- [3] *Faraday Discussions*, 215, 313 (2019).
- [4] *J. Am. Chem. Soc.* 133, 20863 (2011).
- [5] *ChemSusChem* 10, 112 (2017).
- [6] *J. Am. Chem. Soc.* 138, 10260 (2016)

A personal perspective into the catalysts for hydrogen production

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Hydrogen (H₂) has been present incessantly in the modern research's pipeline over the last two decades, being the subject of a massive research. Among the small molecules, the utility of H₂ is perhaps unmatched, being a key chemical for many industrial sectors, used for example in the ammonia synthesis, in hydrogenation reactions towards fine chemicals, and in oil refining. For this reason, the efficient synthesis of H₂ has been tackled (and implemented at industrial level), relying on well-known processes such as steam reforming or coal partial oxidation. In this framework, development of catalytic materials for enhanced H₂ production has been one of the main dragging forces in H₂ research, and some attractive opportunities have been offered by combining production of H₂ with fuel cell technologies, for instance in the context of reducible metal oxide catalytic materials for solid oxide fuel cells (SOFC). In recent years, there has been a progressively increasing interest in using H₂ as a green energy vector, whereby its oxidation is able to power energy without release of greenhouse gases, at least in theory. In order to comply with current sustainability guidelines (CO₂ zero emission), however, the production of H₂ must be itself deriving from environmentally friendly approaches. Water electrolysis is one of the alternative methods to form H₂, where electric current is used to split water into H₂ and O₂, therefore hinting on a carbon neutral footprint. However, potential downsides relate to the source of such electricity, which is typically provided by exploitation of carbon-derived products, hence calling for a careful evaluation of the overall process. A more appealing strategy which has been drawing increasing attention is the use of photocatalysis, and has led to the proliferation of heterogeneous semiconductor catalysts able to form hydrogen by exploiting solar light, through processes based on alcohol photoreforming or in some notable cases on pure water splitting. In this presentation, I will overarch all my years of research on H₂ synthesis via various approaches, from the traditional steam reforming to the electrocatalytic water splitting and photoreforming, highlighting the critical aspects in catalytic material development with purpose-driven functionality.

Sunlight-driven hydrogen formation by membrane-supported photoelectrochemical water splitting

Professor Nathan. S. Lewis

California Institute of Technology
Division of Chemistry and Chemical Engineering
Beckman Institute and Kavli Nanoscience Institute

We are developing an artificial photosynthetic system that will utilize sunlight and water as the inputs and produce hydrogen and oxygen as the outputs. We are taking a modular, parallel development approach in which three distinct primary components—the photoanode, the photocathode, and the product-separating but ion-conducting membrane—are fabricated and optimized separately before assembly into a complete water-splitting system. The design principles incorporate two separate, photosensitive semiconductor/liquid junctions that will collectively generate the 1.7-1.9 V at open circuit necessary to support both the oxidation of H₂O (or OH⁻) and the reduction of H⁺ (or H₂O). The photoanode and photocathode will consist of rod-like semiconductor components, with attached heterogeneous multi-electron transfer catalysts, which are needed to drive the oxidation or reduction reactions at low overpotentials. The high aspect-ratio semiconductor rod electrode architecture allows for the use of low cost, earth abundant materials without sacrificing energy conversion efficiency due to the orthogonalization of light absorption and charge-carrier collection. Additionally, the high surface-area design of the rod-based semiconductor array electrode inherently lowers the flux of charge carriers over the rod array surface relative to the projected geometric surface of the photoelectrode, thus lowering the photocurrent density at the solid/liquid junction and thereby relaxing the demands on the activity (and cost) of any electrocatalysts. A flexible composite polymer film will allow for electron and ion conduction between the photoanode and photocathode while simultaneously preventing mixing of the gaseous products. Separate polymeric materials will be used to make electrical contact between the anode and cathode, and also to provide structural support. Interspersed patches of an ion conducting polymer will maintain charge balance between the two half-cells.

By passing wires – monolithic integrated devices for solar driven hydrogen production and solar batteries

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As we are moving towards a zero-carbon economy, solar will play an integral part in the next generation energy generating and storage technologies. Devices that integrate solar energy conversion and fuel production or storage in one unit are attractive for decentralized deployment where energy generation is in the vicinity of the users. They have the added advantages of smaller footprint and shorter deployment time as the need and cost for the supporting infrastructure (e.g., site preparation, “poles and wires”, transformers amongst others for large scale solar farms or wiring, maximum power point trackers, inverters for conventional roof-top systems) are reduced.

In this talk, I will also talk about design criteria and challenges for low cost, high performance monolithic photovoltaic-electrochemical (PV-EC) devices and our recent work on this using perovskite single junction or tandem solar cells. I will also talk about our recently reported work on integrating high-efficiency perovskite/silicon tandem solar cells with BTMAPVi/NMe-TEMPO redox couples for solar flow battery with record performance.

References

- [1]. H. Chen, M. Zhang, T. Tran, R. Bo, L. Shi, I. Di Bernardo, J. Bing, J. Pan, S. Singh, J. Lipton-Duffin, T. Wu, R. Amal, S. Huang, A. W. Y. Ho-Baillie and A. Tricoli, “Integrating Low-Cost Earth-abundant Cocatalysts with Encapsulated Perovskite Solar Cells for Efficient and Stable Overall Photoelectrochemical Water Splitting”, *Advanced Functional Materials*, adfm.202008245
- [2]. W Li, J Zheng, B Hu, HC Fu, M Hu, A Veyssal, Y Zhao, JH He, TL Liu, A. Ho-Baillie, S. Jin, “High performance solar flow battery powered by a perovskite/silicon tandem solar cell, *Nat. Mater.* 19, 1326–1331 (2020). <https://doi.org/10.1038/s41563-020-0720-x>

TiFe-type intermetallics for large-scale stationary hydrogen storage

Fermin Cuevas^{1,*}, *Erika M. Dematteis*^{1,2}, *David Michael Dreistadt*³, *Giovanni Capurso*³,
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The intermittency of renewable sources requires the use of storage systems to balance energy production and demand. The hydrogen chain “production-storage-conversion” is considered as a key solution. It commonly comprises *i*) hydrogen production by water electrolysis, *ii*) hydrogen storage and *iii*) hydrogen conversion into electrical energy by means of a fuel cell. Hydrogen can be stored in different states: compressed gas, liquefied, or chemically bonded in solid compound such as metallic hydrides. The latter affords reversible hydrogen storage under mild thermodynamic conditions close to room temperature and atmospheric pressure. Metal hydrides offer safe, compact and long-term energy storage, making them well-adapted to stationary applications when using low-cost efficient intermetallic compounds and advanced system integration.

The European project HyCARE (www.hycare-project.eu), running from 2019 to 2022, aims to demonstrate the efficient use of metal hydrides, coupled to phase change materials, to store approx. 50 kg of hydrogen, the highest quantity ever accumulated in Europe following this solid-state approach and combined technology. Among the 10 partners integrating HyCARE, the CNRS leads the tailoring and optimization of the alloy composition work package. It comprises, alloy design, tuning to thermodynamic operation conditions, activation and kinetic issues, as well as to cycling stability, resistance to impurities and limited use of raw critical materials. Based on available data [1], low-cost TiFe-based intermetallic alloys have been selected. Composition and microstructure were optimized in terms of thermodynamics, activation, kinetics and cycle-life [2-3]. Thus, Ti-rich Mn-substituting compounds have been developed and their hydrogen properties deeply characterized by many-fold techniques, including analysis of reversible hydrogen uptake by *in-situ* neutron diffraction. Application of TiFe-based intermetallics in the HyCARE project will be presented together with future prospective for these materials.

Reference

[1] E.-M. Dematteis, N. Berti, F. Cuevas, M. Latroche, M. Baricco, "Substitutional effects in TiFe for hydrogen storage: a comprehensive review", *Mater. Adv.*, 2 (2021) 2524 – 2560. DOI: <https://doi.org/10.1039/D1MA00101A>

[2] E.-M. Dematteis, F. Cuevas, M. Latroche, "Hydrogen storage properties of Mn and Cu for Fe substitution in TiFe_{0.9} intermetallic compound", *J. Alloys Comp.*, 851 (2021) 156075. DOI: <https://doi.org/10.1016/j.jallcom.2020.156075>

[3] E.-M. Dematteis, D. M. Dreistadt, G. Capurso, J. Jepsen, F. Cuevas, M. Latroche, "Fundamental hydrogen storage properties of TiFe-alloy with partial substitution of Fe by Ti and Mn", *J. Alloys Comp.*, 874 (2021) 159925. DOI: <https://doi.org/10.1016/j.jallcom.2021.159925>

H₂ Generation - 1

Session

High efficiency direct solar hydrogen generation

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Combining perovskites with well-established photovoltaic materials such as silicon is an attractive option for producing cheap, high efficiency and high voltage solar cells. Perovskite/silicon tandems also have the potential for producing highly efficient stand-alone direct hydrogen generation systems. We demonstrate 20% efficiency direct solar to hydrogen generation using a low-cost system of perovskite/silicon tandem cells integrated with earth abundant metal catalysts. We also discuss potential end uses of hydrogen production in the context of global trends in renewable energy.

Solar thermochemical water splitting cycle with a particle reactor

Tatsuya Kodama

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The greatly isolated “sun-belt” regions include south-western United States, most of Australia, etc., where direct normal irradiation exceeds 2000 kWh/m²/year. Some modern solar-concentrating systems, such as central tower, and advanced beam-down system, have concentration factors in 1000 –2000 range and can provide high-temperature solar heat of 20–100 MW_{th} or more. Concentrated solar radiation is focused upon a solar receiver/reactor where temperatures may reach 1500°C. A two-step thermochemical water splitting cycle using a redox system of metal oxide is one of the promising solar thermochemical processes to produce H₂. The present author has proposed a novel concept of particle fluidized solar reactor for the two-step water splitting cycle. A fluidized bed of redox metal oxide particles is directly irradiated by concentrated solar radiation in the reactor which has a transparent quartz window on top of the reactor. Concentrated solar radiation passes downward through the window and directly heats the particles in an upper region of the particles fluidized bed. This solar reactor concept needs to be combined with a beam-down (BD) type solar concentrator. Niigata University and University of Miyazaki started an R&D joint project in 2011, to demonstrate the fluidized bed reactor on solar. A new type of 100 kW_{th} BD solar concentrating system with a secondly elliptical reflector was built in 2012 at the campus of University of Miyazaki, Japan. The solar demonstration of the particle fluidized bed reactor was conducted for the two-step water splitting cycle using ceria particles and hydrogen could be produced at Miyazaki BD system. Recently, CSIRO (Australian National Laboratories), Niigata University and the Institute of Applied Energy (Japan) have started the new project “Solar Thermochemical Hydrogen Research and Development” under financial support by Australian Renewable Energy Agency (ARENA). In the project, the fluidized bed reactor is planned to be up-scaled to 300-500 kW_{th} solar energy input scale and demonstrated on solar at the CSIRO Energy Centre in Newcastle NSW, Australia.

Advanced semiconductor and catalytic materials for direct solar hydrogen generation

Siva Karuturi

Australian National University

Solar energy has the greatest potential to replace fossil fuels among all carbon-free energy sources. Given that electricity only accounts for 30% of global energy consumption, breakthroughs in renewable energy storage and transportation are needed to accomplish the transition to renewable energy, along with the development of a supply chain for renewable energy exports. The chemical bonds present in chemical fuels provide one of the densest ways to store energy. For example, energy density of hydrogen fuel is 100 times higher than that of a best Li-ion battery. Hydrogen generated from solar-driven water splitting has the potential to provide clean, sustainable, abundant, and transportable energy. In this talk, I will present on the development of semiconductor photoelectrodes for solar hydrogen generation. Specific strategies to enhance the light harvesting, catalytic activity, and long-term stability of photoelectrodes will be explained in detail. Following this, I will introduce our work on tandem semiconductor systems for spontaneous hydrogen evolution using solar energy as the sole energy input. In particular, our recent results on perovskite/Si tandems for stand-alone water splitting systems achieving high solar-to-hydrogen efficiency will be presented.

Photoelectrochemical applications of chalcopyrite and kesterite compound thin films

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Photoelectrochemical (PEC) conversion of sunlight into a chemical energy of hydrogen (H₂) through water splitting has been studied extensively to achieve production of storable and transportable energy sources from sunlight. Reduction of carbon dioxide (CO₂) using water (H₂O) as an electron source into a more reduced chemical species is also an important subject for utilization of solar energy because of its possible production of energy-rich carbonaceous compounds without the use of fossil resources. Among the various possible systems, a coupling of two different semiconductor electrodes termed a Z-scheme system has been studied as an attractive concept in recent years. For the photocathode side in the Z-scheme system, p-type polycrystalline thin films composed of metal chalcogenides have been studied extensively. Specifically, Cu-containing chalcopyrite and kesterite compounds, which were originally used as photovoltaic materials, have received significant attention due to their long absorption edge wavelengths and their suitable band structures for the reaction. We found that a kesterite Cu₂ZnSnS₄ compound thin film is a promising photocathode for PEC water splitting after appropriate surface modifications were applied.¹ Similar structural controls were also found to be effective for chalcopyrite CuInS₂ and CuGaSe₂ compounds to induce water reduction.² In this presentation, I introduce our developed stable and efficient photocathodes based on these thin film photocathodes with focusing on their micro- and electron-energy structures.

References

- 1) For example, J. Am. Chem. Soc., 137, 13691 (2015); Energy Environ. Sci., 14, 1480 (2021).
- 2) For example, Angew. Chem., Int. Ed., 53, 11808 (2014); ACS Appl. Mater. Interfaces, 7, 16086 (2015).

Photocatalysts for H₂ production based on metal clusters as co-catalysts

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Photocatalysis is one of the pathways to generate H₂ through the use of renewable energy. Highly efficient photocatalysts have been developed for wavelength of 400 nm or shorter.¹ A key aim in this field is to develop efficient photocatalysts that operate at longer wavelength so that a larger part of the solar spectrum can be used.

Metal clusters deposited onto metal oxide surfaces have been shown to act as co-catalysts for H₂ producing photocatalysts.² Metal clusters with a size of less than 100 atoms are suitable for modifying the electronic properties of semiconductor surfaces.³⁻⁴ It is assumed that the function of the cluster in a photocatalyst is based on their unique electronic structure. It is known that the electronic structure of clusters depends on the number of atoms forming the cluster. Thus it is important to maintain the specific size of metal clusters in their role as co-catalyst.

A key component of metal cluster based photocatalysts are overlayers which a) allow to protect metal clusters from agglomeration and b) to reduce the recombination reaction of H₂ and O₂. This contribution will show examples of cluster modified surfaces which are protected by metal oxide layers and their use in photocatalytic reactions.

Reference

- (1) Takata, T.; Jiang, J.; Sakata, Y.; Nakabayashi, M.; Shibata, N.; Nandal, V.; Seki, K.; Hisatomi, T.; Domen, K. Photocatalytic water splitting with a quantum efficiency of almost unity. *Nature* **2020**, *581* (7809), 411.
- (2) Kurashige, W.; Kumazawa, R.; Mori, Y.; Negishi, Y. Au₂₅ cluster-loaded SrTiO₃ water-splitting photocatalyst; preparation and elucidation of the effect of cocatalyst refinement on photocatalytic activity. *Journal of Materials and Applications* **2018**.
- (3) Anderson, D. P.; Alvino, J. F.; Gentleman, A.; Qahtani, H. A.; Thomsen, L.; Polson, M. I. J.; Metha, G. F.; Golovko, V. B.; Andersson, G. G. Chemically-Synthesised, Atomically-Precise Gold Clusters Deposited and Activated on Titania. *Physical Chemistry Chemical Physics* **2013**, *15* (11), 3917.
- (4) Krishnan, G.; Eom, N.; Kirk, R. M.; Golovko, V. B.; Metha, G. F.; Andersson, G. G. Investigation of Phosphine Ligand Protected Au₁₃ Clusters on Defect Rich Titania. *J. Phys. Chem. C* **2019**, *123* (11), 6642.

Solid oxide electrolyzers: efficient technology for production and utilization of renewable chemicals and fuels

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Penetration of renewables in energy sector is rapidly growing for the decarbonisation of various energy sectors. However, the intermittent nature of renewables causes several challenges for adoption in existing infrastructure. Storing surplus renewable energy in the form of chemical and fuels is being considered a viable option to provide stable electricity whenever required and also for transportation of energy over long distances to areas lean in renewables. Solid oxide electrolyzers (SOE) are efficient for production of various fuels such as hydrogen, carbon monoxide and/or syngas which once integrated with downstream processes can also produce multiple value-added fuels and chemicals such as methane, olefins and paraffins.^{1,2} SOE are scalable and can be integrated with downstream processes such as ammonia and methanol synthesis.³ Advantageously, waste heat from exothermic synthesis reactors can be utilized in solid oxide electrolyzers which could lower the electric energy input upto 30% for SOE operation and therefore can boost the overall energy efficiency of the system to above 70%. In our recent project funded by ARENA, we have developed SOE materials and cell designs for efficient generation of fuel gases with electric energy input < 40 kWh/kg of hydrogen. This will provide a significant cost reduction for the production of hydrogen in comparison to polymer electrolyte membrane and alkaline electrolyte membranes based technologies (>50 kWh/kg of hydrogen) and makes SOE technology more attractive to achieve DOE target of <\$2/kg of hydrogen. This talk will present the overview of SOE technology developed at CSIRO, in addition to the integration aspects of the technology with various upstream and downstream processes.

Keywords: Electrochemical energy system, energy storage, renewables, high temperature, steam electrolysis

References

- ¹ S. D. Ebbesen, S. H. Jensen, A. Hauch, and M. B. Mogensen. *Chemical Reviews* 2014, *114*, 10697–10734.
- ² G Kaur, A P Kulkarni, D Fini, S Giddey, A Seeber. *Journal of CO₂ Utilization* 2020, *41*, 101271.
- ³ A P Kulkarni, T Hos, M V Landau, D Fini, S Giddey, M Herskowitz. *Sustainable Energy & Fuels* 2021, *5*, 486-500.

H₂ Carrier - 1

Session

Towards solar fuels – hydrogen and ammonia

Professor Doug MacFarlane

School of Chemistry, Monash University

In current discussions of new industries for Australia and a path to a zero net carbon future, "green hydrogen" – producing hydrogen fuel using renewable energy – features prominently. The dream is capturing Australia's abundant but variable renewable resources – wind and sunshine – in a storable and transportable (and exportable) form. What does it involve? How can it be done? Is it feasible? How can it be used? Are there any other similar fuels? Ammonia? This talk will open up a discussion of the concepts, the issues and the possible solutions, including the production and use of ammonia as an energy carrier and fuel.



Process considerations for electrochemically driven green ammonia and carbon negative materials

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Electrochemical engineering is the next frontier in clean manufacturing as it allows chemical processes to be driven with renewable electricity. Electrification of manufacturing is necessary in order to decarbonise a multitude of essential processes including steel making and ammonia generation. Use of renewable energy to drive carbon capture and utilisation (CCU) is also an important future area which will enable technology solutions to offset emissions in areas where fossil fuel elimination is difficult (such as agriculture). Here electrochemically driven manufacturing processes will be outlined and considerations for integration of each process with renewable energy considered, shown in Figure 1.

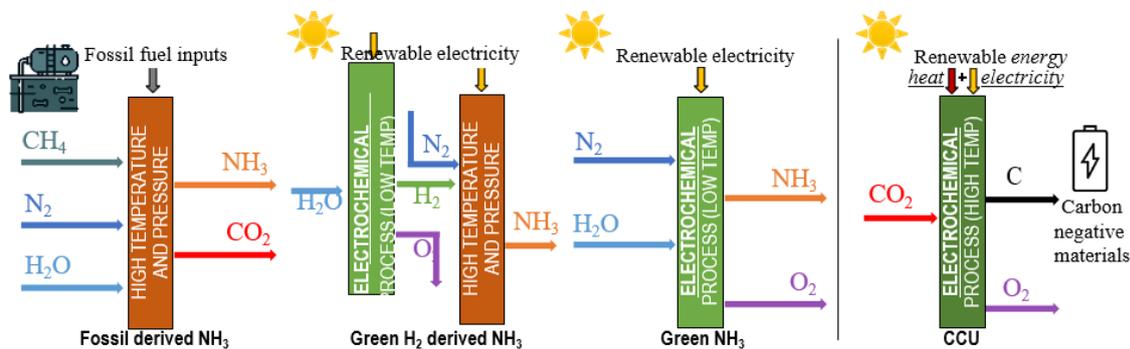


Figure 1. Electrochemical processes for net-zero emission manufacturing

Ammonia production is currently driven by fossil fuels. There is great interest using renewable hydrogen instead, generated electrochemically. It is also possible to directly generate ammonia electrochemically and substantial research work has been done in this area to enable electrochemical ammonia formation. Work presented here will show that balance of plant requirements for electrochemically driven ammonia formation can match the energy demand for the generation itself, and careful consideration of processing and separation is required for a practical solution. The power to ammonia requirement for the electrochemical process was estimated at 23 kWh.kg NH₃⁻¹ [1] compared to ~13 kWh.kg NH₃⁻¹ for green hydrogen approach and ~10 kWh.kg NH₃⁻¹ for traditional Haber-Bosch.

Carbon capture and utilisation (CCU) is also an important future area for achieving net-zero emissions. Converting carbon dioxide into useful, stable products requires substantial energy inputs. Using high temperature electrolysis can enable formation of stable and useful carbon products, however requires both thermal and electrical energy. Here, integration of the electrolysis unit with concentrated solar thermal energy is proposed [2] with validated end-use cases for the high value carbon product generated [3].

References

- [1]. J. Allen, S. Panquet, A. Bastiani (Submitted, Aug '21), "Electrochemical ammonia: Power to ammonia ratio and balance of plant requirements for two different electrolysis approaches", *Front. Chem. Eng*
- [2]. J. Allen (2019). "Renewable carbon for energy storage". In: *WEC2019: World Engineers Convention 2019*. Melbourne: Engineers Australia, 2019: 1707-1714. Engineers Australia.
- [3]. J. Wu, S. Moradmand, W. K. Pang, J. Allen and N. Sharma (2021). "Sodium-ion battery anodes from carbon depositions." *Electrochimica Acta* 379: 138109.

Amine-borane systems featuring room temperature dehydrogenation

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Abstract: Amine-borane complexes have been extensively studied as hydrogen storage materials. Recently, we have discovered new reactions between these complexes and amines generating high purity H₂ gas under ambient conditions. For example, the reaction between ethylenediamine bisborane (EDAB) and ethylenediamine (ED) leads to unique boron-carbon-nitrogen 5-membered rings in the dehydrogenation product where one boron is tri-coordinated by three nitrogen atoms. Due to the unique cyclic structure, the dehydrogenation product can be efficiently converted back to EDAB by NaBH₄ and H₂O at room temperature. Several other systems will be discussed as well. These findings further demonstrate the potential of amine boranes as hydrogen storage materials.

Reference

G. Zhang, D. Morrison, G. Bao, H. Yu, C. W. Yoon, T. Song, J. Lee, A. T. Ung, Z. Huang, *Angew. Chem. Int. Ed.*, 2021, 60, 11725–11729.

Y. Zhu, L. Ouyang, H. Zhong, J. Liu, H. Wang, H. Shao, Z. Huang, M. Zhu, *Angew. Chem. Int. Ed.*, 2020, 59, 8623-8629.

Z. Huang, S. Wang, R.D. Dewhurst, N. V. Ignat'ev, M. Finze, H. Braunschweig, *Angew. Chem. Int. Ed.*, 2020, 59, 8800 – 8816.

Methane as a renewable energy carrier

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Synthesis of methane from renewable H₂ and ambient CO₂ can be of great interest to Australia, due to its abundant renewable energy resources, the readily available infrastructure for gas export and its potential to compete with the emerging energy intensive liquid hydrogen export counterpart. The integration of CO₂ capture from ambient air (DAC) process and CO₂ methanation using the Sabatier reaction can be considered as a net zero emission technology because the energy requirement of the DAC process can be provided by the high-quality heat released from methanation reactions.

As an alternative to the available DAC technology from commercial providers such as Climeworks, Global Thermostat and Carbon Engineering, the DAC system can also use an amine-based solution. Amine solutions are the leading technology for CO₂-capture from flue gases due to the ease of scalability of the technology. This is of considerable benefit and relevance to DAC as well. Moreover, the abundant availability of design and cost information often embodied in available process modelling tools ensures that techno-economic assessments can be carried out conveniently and deliver credible results.

In this work, a techno economic analysis of the production of liquified synthetic methane from ambient CO₂ and renewable hydrogen was conducted. An initial process design and techno-economic assessment was made using as a standard absorbent solution incorporating mono-ethanolamine. Subsequently, process improvements focused on reducing major cost components were introduced. These included the introduction of low volatility amines and replacement of the steel absorber column materials by cheaper plastic materials, widely used in cooling towers. The process improvements were evaluated through process modelling (DAC and methanation) and an extensive technology qualification program targeting the amine-based DAC process. This formed the basis for an overall process design that was used for the cost analysis.

The presentation will provide a comprehensive overview of the work conducted, its results, conclusions, and recommendations for next steps.

Efficient solar-to-hydrogen conversion process enabled by photovoltaic electrolysis

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Photovoltaic electricity powered water electrolysis provides an appealing solution to produce the green hydrogen fuel (H₂) from abundant solar energy¹, facilitating the curb of global CO₂ emission that benefits a sustainable future. However, the practical efficacy of this technology is severely limited by the low solar-to-hydrogen (STH) conversion efficiencies, which are mainly caused by the unsatisfactory performance of water electrolyzers and photovoltaic devices that leads to a mismatch between these two systems². To this end, the development of an efficient photovoltaic electrolysis (PVE) system with a high STH efficiency is of paramount significance. Herein, we designed an efficient PVE system that integrates a state-of-the-art concentrated photovoltaic (CPV) device with a cost-effective alkaline water electrolyser. By employing an efficient heat exchange system, the thermal energy produced from the CPV device could be used effectively to heat the electrolyte in water electrolysis system, boosting the water splitting performance at an elevated temperature. Moreover, the high-performance anodic oxygen evolving catalyst, an iron/nickel composite, designed in this work also enables a high H₂ conversion efficiency of water electrolyser at large operation currents (e.g., 1 to 10 A). As a result, the as-developed PVE system makes a full utilization of electricity and heat energy generated from the CPV cells without sacrificing the water electrolysis performance, giving high STH efficiencies under practical H₂ productivities.

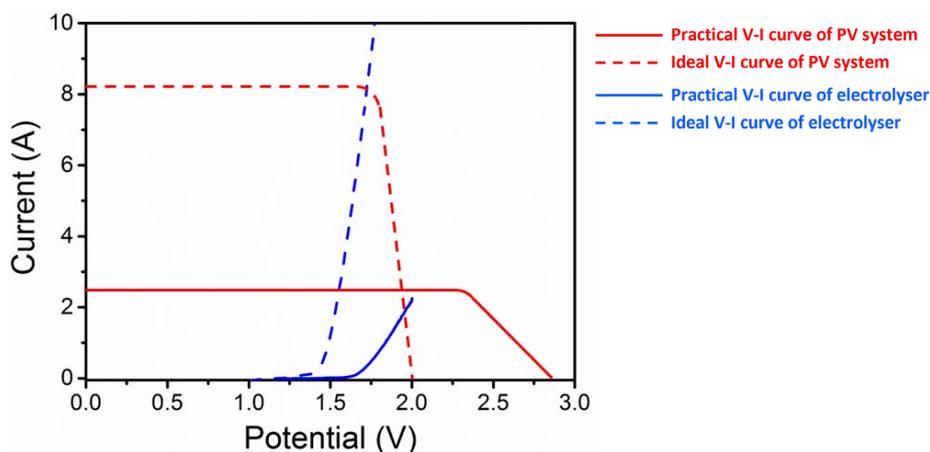


Figure 1: The I-V curves of the photovoltaic (red lines) and electrochemical components (blue lines).

References

- (1) Jia, J.; Seitz, L. C.; Benck, J. D.; Huo, Y.; Chen, Y.; Ng, J. W. D.; Bilir, T.; Harris, J. S.; Jaramillo, T. F. Solar Water Splitting by Photovoltaic-Electrolysis with a Solar-to-Hydrogen Efficiency over 30%. *Nat. Commun.* **2016**, *7* (1), 13237. <https://doi.org/10.1038/ncomms13237>.
- (2) Tembhurne, S.; Nandjou, F.; Haussener, S. A Thermally Synergistic Photo-Electrochemical Hydrogen Generator Operating under Concentrated Solar Irradiation. *Nat. Energy* **2019**, *4* (5), 399–407. <https://doi.org/10.1038/s41560-019-0373-7>.

H₂ Carrier - 2

Session

Towards sustainable electrosynthesis of hydrogen and ammonia

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Hydrogen and ammonia are important commodity chemicals that are now also broadly considered as the major energy carriers of the future. Both can be produced through sustainable electrochemical processes entirely powered by renewable energy, but these technologies require improvements to take over the traditional methods. Realistically, synthesis of ammonia will still rely on the Haber-Bosch technologies for a reasonable period of time, but will now use increasing amounts of H₂ derived from water electrolysis, which will substantially decrease the CO₂ footprint of the NH₃ production. Moreover, the current best electrochemical ammonia generation systems also require pure hydrogen as the source of protons and electrons. This further emphasises the strategical importance of the development of scalable electrochemical water splitting technologies.

The presentation will discuss possible strategies towards further improvements in the sustainable H₂ + NH₃ production technologies and will present some of the recent developments in the field from our group. In the H₂ domain, the focus will be on new anode catalytic systems and concepts for the acidic water splitting that can potentially overcome the limitations of the current best polymer electrolyte designs. With respect to the NH₃ electrosynthesis, our progress towards the development of stable high-performance systems operating via a redox mediated mechanism will be presented. In conclusion, a perspective on possible future directions that are likely to further advance the presented technologies and the overall concept of the Ammonia Economy for the future energy will be discussed

Hierarchically structured catalysts for sustainable energy production

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Concerns over the economics of proven fossil fuel reserves, and global acceptance of the anthropogenic origin of rising CO₂ emissions and associated climate change from combustible carbon, is driving the quest for new routes to sustainable energy sources.¹ Catalysis has a rich history of facilitating energy efficient, selective molecular transformations,² and in a post-petroleum era will be pivotal role in overcoming the scientific and engineering barriers to sustainable and economically viable energy vectors. Here we outline challenges in the design and application of catalytic technologies for the upgrading of lignocellulosic biomass to liquid transportation fuels.

Advances in the rational design of nanoporous solid acid and base catalysts, possessing hierarchical architectures³ or tailored surface functionality, enables energy efficient esterification and transesterification of bio-oil components into biodiesel. Judicious compartmentalisation of different active sites within hierarchical porous frameworks (**Figure 1**) permits biodiesel production from low grade oil feedstocks which cannot be processed by current commercial technologies.⁴ Synergies between hierarchical solid acids and metal nanoparticles also facilitate active and selective upgrading of phenolic components of pyrolysis bio-oils to hydrocarbon fuels, and precious metal thrifting.⁵

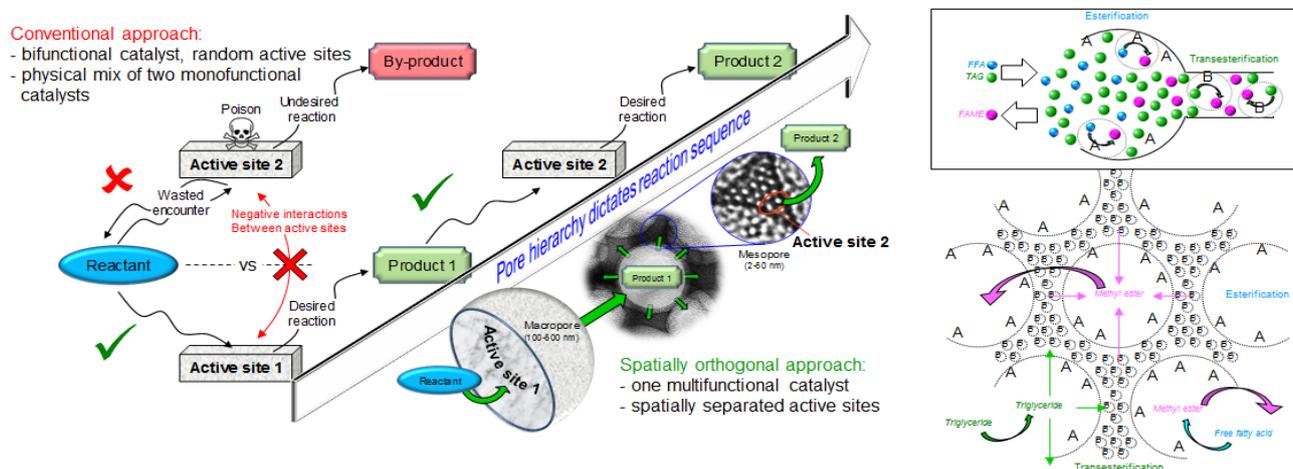


Figure 1: Spatially orthogonal acid-base catalyst for the one-pot production of biodiesel from low grade oil.

References

¹ Chu, S.; Majumdar, A. *Nature* 2012, 488, 294.

² Zhang, X.; Wilson, K., Lee, A.F. *Chem. Rev.* 2016, 116, 12328.

³ Parlett, C.M.A.; Isaacs, M.A.; Beaumont, S.K.; Bingham, L.M.; Hondow, N.S.; Wilson, K.; Lee, A.F. *Nature Mater.* 2016, 15, 178.

⁴ Isaacs, M.A.; Parlett, C.M. A.; Robinson, N.; Durndell, L.J.; Manayil, J.C.; Beaumont, S.K.; Jiang, S.; Hondow, N.S.; Lamb, A.C.; Jampaiah, D.; Johns, M.L.; Wilson, K.; Lee, A.F. *Nat. Catal.* 2020, 3, 921.

⁵ Shivhare, A.; Hunns, J. A.; Durndell, L. J.; Parlett, C.M.A.; Isaacs, M.A.; Lee, A. F.; Wilson, K. *ChemSusChem* 2020, 13, 4945.

Controlling electrolyser flooding at high-current density in electrochemical CO₂ conversion to CO and ethylene

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Highly efficient and selective catalysts are demonstrated in lab-scale CO₂ reduction reaction (CO₂RR) studies⁵⁻⁷, but one of the crucial reasons that these advances in catalyst materials are not fully realised in large-scale CO₂RR technologies is the slow rates of CO₂ transport from the bulk gas to the electrolyte-catalyst interface where the CO₂ reduction reaction (CO₂RR) occurs.⁸ Continuous CO₂RR electrolysers with gas diffusion electrodes (GDEs) can overcome the CO₂ mass transport limitations to achieve industrially relevant reaction rates at current densities above 200 mA cm⁻².⁹

However, two key problems experienced at these conditions are (i) that liquid electrolyte *floods* the gas diffusion layers, which impedes the diffusion of CO₂ into and gas products out of the electrolyser; and (ii) the wetting state of the catalyst layer (CL) depends on charged state and in turn can affect local reaction conditions at the electrolyte-catalyst interface¹⁰. In *Linkage Project LP160101729* we observed the practical implications of GDE flooding which constrain the maximum current density and reduce product selectivity. In this presentation we will share recent work to understand how electrode structure affects flooding during CO₂ electrolysis, and approaches to mitigate flooding by modification of the carbon substrate (microporous layer) and the catalyst layer in the GDE. These approaches include adding different carbon nanomaterials to the GDE support and optimising the ionomer-solvent ink used to deposit the catalyst particles on the electrode.

References

1. Li, F., et al., *Nanoscale* **2018**, *10* (14), 6235-6260.
2. Yang, W., et al., *Advanced Materials Technologies* **2018**, *0* (0), 1700377.
3. Ziqi, T., et al., *Advanced Theory and Simulations* **2018**, *1* (5), 1800004.
4. Garg, S., et al., *Journal of Materials Chemistry A* **2020**, *8* (4), 1511-1544.
5. Burdyny, T.; Smith, W. A., *Energy & Environmental Science* **2019**, *12* (5), 1442-1453.
6. Li, M., et al., *Journal of Materials Chemistry A* **2021**.

Heterogeneous molecular electrocatalysts for carbon dioxide reduction in water

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Electrochemical reduction of CO₂ to CO in water catalysed by low-cost molecular catalysts is a viable way to environmentally friendly CO₂ valorisation, while efficient catalyst immobilization on the electrode surface is one of the key challenges to answer. Herein we present a concept of “molecular wire” i.e. connection of the catalyst to electrode via a conductive covalent linker, which has profound effect on electrocatalytic performance compared to the noncovalent mode. Variable frequency square wave voltammetry results demonstrate that the electron transfer from electrode onto the moiety plays an important role in overall redox kinetics and conductive link with the support is a key element of heterogeneous catalyst design. However, their low stability under negative potentials calls for development of novel stabilization strategies. Mechanistic studies reveal that the deactivation of Co porphyrins during CO₂ reduction proceeds via two major pathways. The first mechanism involves reductive carboxylation while the second one yields inactive oxidized Co^{III} species. We further demonstrate that the thermodynamic inhibition of the reductive pathway could be achieved via introduction of bulky donating substituents into lateral aromatic groups.

References

- [1] E. E. Benson, C. P. Kubiak, A. J. Sathrum, J. M. Smieja, *Chem. Soc. Rev.* 2009, 38, 89.
- [2] C. Costentin, M. Robert, J.-M. Saveant, *Chem. Soc. Rev.* 2013, 42, 2423.
- [3] A. Marianov, Y. Jiang, *Appl. Catal. B* 2019, 244, 881.
- [4] A. Marianov, A. Kochubei, T. Roman, O. Conquest, C. Stampfl, Y. Jiang, *ACS Catal.* 2021, 11, 3715.
- [5] A. Marianov, A. Kochubei, T. Roman, O. Conquest, C. Stampfl, Y. Jiang, *Anal. Chem.* 2021.

Pathways to light assisted CO₂ activation and potential application in solar thermal carbon capture and utilisation.

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Carbon capture and utilisation is one of the strategies to manage the detrimental contribution of CO₂ to climate change. Direct utilisation of solar power provides a feasible technical solution to the energy-intensive up-convert carbon dioxides into active carbon feedstocks provides a feasible technical solution to solve the energy-intensive CO₂ activation process. While illumination has shown beneficial synergy benefits in CO₂ hydrogenation, it is unclear whether it is only (i) a simple heating effect or (ii) the light partake directly in the reaction. To complicate things further, the hydrogenation of CO₂, e.g. the Sabatier reaction,¹ while represented by a simple equation (1), undergoes multiple intermediary transitions represented by equation (2).



Over the years, we have created systems in which one of the effects plays a dominant role in the light enhancement effect. In one of the most important findings, we directly observed the interaction of light with the adsorbed formate, HCO₂^{*} species.² This observation was made possible by combining steady-state isotopic kinetic analysis and diffuse reflectance infrared Fourier transform spectroscopy. This finding enables the better creation of conducive environments for light-adsorbate interaction by promoting: (i) support adsorptivity and (ii) metal-support interaction. In particular, this approach was applied to methanol synthesis, equation (3), whereby the formation of HCO₂^{*} is known to occur.^{3,4} In addition to the fundamental studies, we are scaling the solar thermal reactor and identifying solvable engineering issues with this process.



Reference

¹ Sabatier, P.; Senderens, J.-B. *Comptes rendus* 1902, 134, 689–691.

² Tan, T. H.; Xie, B.; Ng, Y. H.; Abdullah, S. F. B.; Tang, H. Y. M.; Bedford, N.; Taylor, R. A.; Aguey-Zinsou, K.-F.; Amal, R.; Scott, J. *Nat. Catal.* 2020.

³ Xie, B.; Wong, R. J.; Tan, T. H.; Higham, M.; Gibson, E. K.; Decarolis, D.; Callison, J.; Aguey-Zinsou, K.-F.; Bowker, M.; Catlow, C. R. A.; Scott, J.; Amal, R. *Nat. Commun.* 2020, 11 (1), 1615.

⁴ Xie, B.; Kumar, P.; Tan, T. H.; Esmailpour, A. A.; Aguey-Zinsou, K.-F.; Scott, J.; Amal, R. *ACS Catal.* 2021, 5818–5828.

H₂ Storage Sessions

Is there a role for metal-hydride hydrogen storage in the developing hydrogen economy?

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The original drive for metal hydride hydrogen storage was in relation to vehicles, but that was overtaken by pressurised gas because the materials are too heavy or operationally intractable. There are other niches, including storage for off-grid energy systems and MH hydrogen compressors. I could say something about these, as well as some of the underlying issues that affect the prospects for commercial rollout of MH technologies. I would normally include at minimum an overview slide that puts MH storage into context compared to pressurised gas, but depending where I am in the program and the duration of the slot could say more on hydrogen storage generally if appropriate.

Options for Underground Storage of Hydrogen in Australia

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Widespread adoption of hydrogen in Australia as an energy carrier will require storage options to buffer the fluctuations in supply and demand, both for domestic use and for export. Once the scale of storage at a site exceeds tens of tonnes, underground hydrogen storage (UHS) is the preferred option for reasons of both cost and safety.

UHS in salt caverns (created by circulation of water) is an established technology internationally, with individual sites able to store a few thousand tonnes of hydrogen. Various Australian sedimentary basins contain salt deposits potentially suitable for the creation of storage caverns; however, most of these salts are in areas that are not near potential hydrogen generation, ports or processing infrastructure. The most likely locations are in the north-western part of the Canning Basin in Western Australia, the Adavale Basin in western Queensland, and the Amadeus Basin in the Northern Territory.

Depleted gas fields have also been used previously for storage of hydrogen-rich gas mixtures as well as natural gas storage and appear to be the most promising and widely available UHS option in Australia. There are still technical challenges to be addressed, such as the extent of possible contamination of the stored hydrogen with residual hydrocarbons, and the possible effects of geochemical reactions and microbial processes. The total prospective UHS capacity in such sites has been estimated to be 310 million tonnes. Even if only a small fraction of this prospective storage capacity could be realised commercially, this would significantly exceed the storage needs of a fully developed hydrogen industry in Australia (estimated at around 5 million tonnes). Saline aquifers and engineered hard-rock caverns provide additional storage options, although these are less established and may only need to be pursued in cases where salt caverns or depleted fields are not available.

MBNH materials for solid-state hydrogen storage – Focus on alkali and alkaline-earth hydrazinidoboranes

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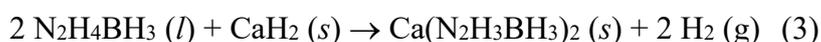
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With ammonia borane NH_3BH_3 as the leading compound,¹ BNH materials have shown to be attractive solutions for solid-state hydrogen storage, though they do not allow storing H_2 in a reversible way at suitable operating conditions.² BNH materials are none other than derivatives of ammonia borane. One example is hydrazine borane $\text{N}_2\text{H}_4\text{BH}_3$.³ Other examples are the alkali and alkaline-earth derivatives of ammonia borane as well as of hydrazine borane, which are amidoboranes and hydrazinidoboranes, also denoted MBNH materials.⁴ Few years ago, we focused our attention on the hydrazinidoborane derivatives. As a first step, we synthesized and fully characterized the alkali compounds $\text{MN}_2\text{H}_3\text{BH}_3$ by reacting hydrazine borane with the corresponding metal hydride (Eq. 1),³ or the corresponding metal (Eq. 2):⁵



More difficult has been to succeed in getting the alkaline-earth counterparts $\text{M}(\text{N}_2\text{H}_3\text{BH}_3)_2$. The calcium derivative cannot be obtained by simply milling calcium hydride CaH_2 and hydrazine borane. A subsequent heat-treatment ($<70^\circ\text{C}$), to make the borane be liquid, is required. In doing so, crystalline calcium hydrazinidoborane $\text{Ca}(\text{N}_2\text{H}_3\text{BH}_3)_2$ is obtained:⁶



Currently we are working on the magnesium derivative $\text{Mg}(\text{N}_2\text{H}_3\text{BH}_3)_2$. After a high number of unsuccessful attempts,⁴ we have been able to get the targeted compound.⁷ This work is still being finalized... and, the 4th *Energy Future Conference and Exhibitions 2021* is an excellent opportunity where I will give an overview of our achievements about alkali and alkaline-earth hydrazinidoboranes as potential solid-state hydrogen carriers, with a special focus on the last discovered calcium and magnesium derivatives.

References

- ¹ Demirci, U.B. *Int. J. Hydrogen Energy* **2017**, *42*, 9978-10013.
- ² Kumar, R.; Karkamkar, A.; Bowden, M.; Autrey, T. *Chem. Soc. Rev.* **2019**, *48*, 5350-5380
- ³ Moury, R.; Demirci, U.B. *Energies* **2015**, *8*, 3118-3141.
- ⁴ Castilla-Martinez, C.A.; Moury, R.; Demirci, U.B. *Int. J. Hydrogen Energy* **2020**, under review.
- ⁵ Castilla-Martinez, C.A.; Granier, D.; Charmette, C.; Maurin, G.; Yot, P.G.; Demirci, U.B. *Int. J. Hydrogen Energy* **2019**, *44*, 28252-28261.
- ⁶ Ould-Amara, S.; Yada, V.; Petit, E.; Maurin, G.; Yot, P.G.; Demirci, U.B. *Int. J. Hydrogen Energy* **2020**, *45*, 2022-2033.
- ⁷ Castilla-Martinez, C.A.; Demirci, U.B. *Int. J. Hydrogen Energy* **2020**, to be submitted.

Hydrogen Generation and Storage: from Materials to Components

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Hydrogen is the ideal clean energy carrier for our future sustainable energy economy as well as for zero-emission mobility. Recent research on materials for efficient renewable production 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.

Photocatalysts can be used for water splitting in photo-electrochemical cells. Respective TiO_2 , BiVO_4 , Fe_2O_3 , or WO_3 coatings can be produced by kinetic spraying. In kinetic spraying, particles are accelerated in a gas stream to velocities of more than 800 m/s and bond to the substrate upon impact without additional binding agents. The surfaces show high photo-current for hydrogen production by solar water splitting. Current results on basic mechanisms are presented, and new findings regarding stability of thin TiO_2 -coatings as protection against corrosion are presented.

With respect to hydrogen storage, solid nanostructured hydrides offer a safe and energy efficient solution for stationary as well as mobile applications. Highest energy efficiencies can be achieved, if working temperature and reaction enthalpy of the respective hydrogen releasing process can be tailored for the particular system integration, e.g., with a fuel cell. Tuning of reaction enthalpies can be facilitated using Reactive Hydride Composites (RHC), which release or store hydrogen by redox reactions between at least two hydrides.

H₂ Generation - 2

Session

Solar Fuels from Photocatalysis

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Photocatalytic and photoelectrochemical processes employing photoactive semiconductors are two key systems in harvesting sunlight for energy and environmental applications. Strategies have been formulated to improve the properties of the semiconductor for better performances. However, requirements to yield excellent performances are different in these two distinctive systems. Understanding of the underlying mechanism for the photoexcited charge transportation in relation to their photoactivities is of fundamental importance for rational design of high-performing photoactive materials, which may serve as a useful guideline for the fabrication of good photocatalysts or photoelectrodes toward sustainable solar fuels generation. Many photoactive semiconductors are having inadequate charge transport properties such as low charge mobility, short lifetime, and slow surface kinetics. Standalone single photoactive semiconductors also faces the challenge of meeting the needs for large redox potentials with a sufficiently narrow bandgap for visible light absorption. Coupling two or more components into a photoactive composite may address some of these drawbacks by utilizing the strengths of the individual semiconductors. In this presentation, the charge transportation behavior of single component photoactive semiconductor and composite materials will be examined and discussed (example of BiVO₄ photocatalyst in **Figure 1**).^{1,2} Some new insights on the traditional perception of composite photocatalyst will be shared.

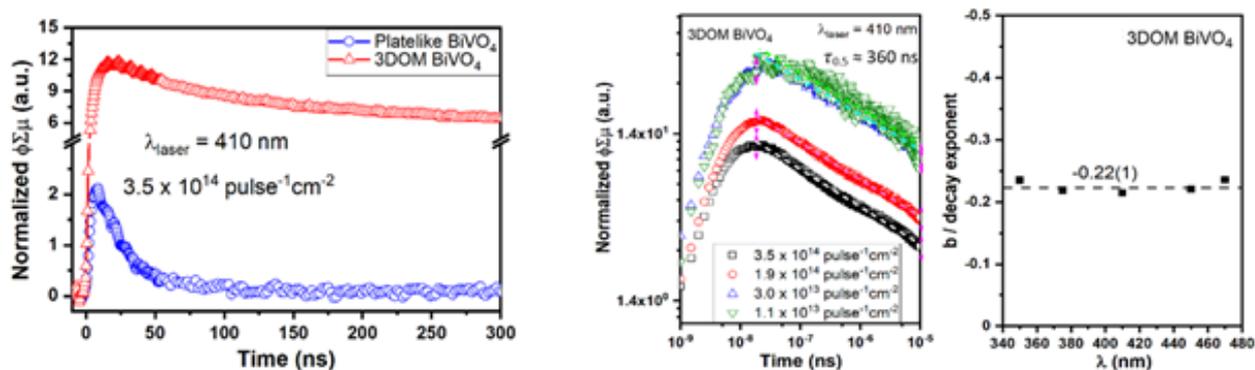


Figure 1. Time-resolved microwave conductivity (TRMC) spectroscopy signals measured for BiVO₄ and its Power-law decay fittings.

References

- 1 H. Wu, R. Irani, K. Zhang, L. Jing, H. Dai, H. Y. Chung, F. F. Abdi, Y. H. Ng*, Unveiling Carrier Dynamics in Periodic Porous BiVO₄ Photocatalyst for Enhanced Solar Water Splitting. *ACS Energy Lett.* 2021, 6, 3400-3407.
2. H. Wu, X. Y. Kong, X. Wen, S. -P. Chai, E. C. Lovell, J. Tang, Y. H. Ng*, Metal-organic Framework Decorated Cuprous Oxide Nanowires for Long-lived Charge Applied in Selective Photocatalytic CO₂ Reduction to CH₄. *Angew. Chem. Int. Ed.* 2021, 60 (15), 8455-8459.

A New Class of Bubble-Free Water Electrolyzer that is Highly Energy Efficient

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Highly efficient electrochemical splitting of water into hydrogen and oxygen constitutes the most critical capability needed for the development of a future hydrogen economy based on renewable energy. In this work we describe a new class of water electrolyzer that directly converts water into hydrogen and oxygen gas, without the need to form gas bubbles on the electrodes. The ‘bubble-free’ nature of the process significantly decreases the energy required. At 80 °C (E°_{cell} 1.18 V), when configured as an alkaline system, the electrolyzer requires a mere 1.52 V to produce hydrogen at 500 mA/cm². This equates to 97% energy efficiency relative to the higher heating value of hydrogen, HHV. The best comparable commercial alkaline electrolyzer cell is only 83% energy efficient under the same conditions, which is 15% lower. Moreover, the *balance of plant* of the new electrolyser is less complex and less energy-hungry than commercial electrolysers. With the improved energy consumption of the balance of plant, the new electrolyser can viably operate at an overall (system) energy efficiency of up to 95%. This is ~20% more energy efficient than any present-day commercial electrolyser.

Optimising Biohydrogen Production in Bacteria using Synthetic Biology

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Microorganisms are able to both synthesize and utilize molecular hydrogen using metalloenzymes known generally as hydrogenases. Two metal ions are usually found in the hydrogenase active sites, with the majority of hydrogenases utilizing Ni^{2+} and/or Fe^{2+} coordinated with both the protein and other small molecules. The assembly of the active site metal complex can require a number of accessory proteins in order to produce a functional enzyme. Fe-Fe hydrogenases found in algae, protists and bacteria are generally used as electron sinks to reduce H^+ and generate H_2 . These Fe-Fe hydrogenases only require two to three maturation proteins to produce a functional hydrogenase, which is in contrast to Ni^{2+} containing hydrogenases, can require up to 20 accessory subunits. By utilizing an algal Fe-Fe hydrogenase in a bacteria or yeast, hydrogen gas can potentially be produced at high rates and good yields from renewable carbon source feedstocks such as sucrose or starch, even without requiring strict anaerobic conditions. We use a synthetic biology approach to engineer bacteria that can efficiently and rapidly convert sugars into hydrogen. This project is funded by the Australian Renewable Energy Agency (ARENA), together with Bioplatforms Australia and BOC Australia.

Understanding Hydrogen Autoignition and Knocking in Spark-Ignition IC Engines

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The use of hydrogen as an alternative fuel in internal combustion (IC) engines poses several challenges and opportunities. Whilst hydrogen's wide flammability limits and its carbon-free chemical structure provide an opportunity to achieve ultra-low, engine-out emissions, its propensity for abnormal combustion could give rise to serious operational challenges. This is particularly the case for engine operation under high power demands, where engine knock is more likely to occur. This work, therefore, investigates hydrogen combustion and its resistance to autoignition in a research spark-ignition (SI) engine.

Our octane rating tests based on the ASTM standard indicate that hydrogen's resistance to end-gas autoignition falls drastically as the in-cylinder charge gets richer in fuel, suggesting that hydrogen-fuelled SI engine is highly knock-prone. Whilst this trend is supported by our detailed in-cylinder pressure measurements, they however show that hydrogen's autoignition resistance is considerably higher than that indicated by conventional standard tests. This finding has significant implications for designing highly efficient hydrogen-fuelled IC engines for power systems and propulsion.

2D materials-based hybrid electrocatalysts for hydrogen generation

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Green hydrogen using renewable electricity is critical for a sustainable energy future, yet its widespread application is hampered by the high cost and scarcity of noble metal-based electrocatalysts. Here we present a range of hybrid electrocatalysts based on 2D materials, which comprise of transition metal dichalcogenides (TMDs) or layered double hydroxides (LDHs) on vertical graphene (VG), for both hydrogen evolution reactions (HER) and oxygen evolution reactions (OER). Superior HER performance with overpotential of 128 mV at 10 mA/cm² and Tafel slope of 50 mV/dec is obtained on MoS₂/VG [1], while OER performance with a mass current of 4.51 A/g (at overpotential of 300 mV) and turnover frequency of 4.8 /s (at overpotential of 400 mV) is obtained on NiFe/VG [2]. Moreover, a bifunctional catalyst of NiCo LDHs/VG is developed for overall water splitting, delivering a cell voltage of 1.66 V at a current density of 10 mA/cm² in 1 M KOH alkaline electrolyte [3]. The group of 2D materials-based hybrid electrocatalysts could thus open new opportunities for low-cost and high-efficiency electrochemical hydrogen production.

References

- [1]. J. Catal. 382: 320 (2020).
- [2]. ACS Nano 14: 11327 (2020).
- [3] Chem. Eng. J. 415: 129048 (2021).

H₂ Applications Sessions

Emerging roles for hydrogen in decarbonizing heavy industrial processes

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The transition toward the net-zero CO₂ production of carbon-intensive products such as steel, aluminium and cement, is driving new markets that are likely to have very significant impacts both on the supply chains for these commodities and on the demand for net-zero hydrogen, green electricity and other low-carbon fuels. It will foster a shift in the locations at which the energy-intensive and carbon-intensive steps in these manufacturing process occur toward those with a coincidence in the availability of both the ore and sources of net-zero hydrogen. The best established pathways to net-zero steel production will employ hydrogen in the iron-making process. In addition, hydrogen is also likely to play a role in the production of low-carbon alumina and cement. However, unlike coal, hydrogen is relatively expensive to transport and store, which makes it desirable to co-produce it with the hydrogen-intensive products within the supply chains for low-carbon metals and construction materials. A wide range of new technologies are therefore emerging to meet the need for these new green products, both in new hydrogen production technologies and in their incorporation into high temperature industrial processes, each of which must be tailored and optimised for the ores and conditions of each location. The presentation will explore these drivers and address some of these important emerging technologies.

H2Xport Project – A Pilot Scale Renewable Hydrogen Plant

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There is significant interest in hydrogen energy for decarbonising the electricity and transport industries to enable the commitments toward climate neutrality and net zero emissions while achieving the UN Sustainability Development Goals. There is a new export demand for hydrogen energy to regions that are deficient in renewable energy. This demand along with the substantial technological progress in fuel cells and lower cost of renewables such as solar is creating a rapid growth in the hydrogen energy industry.

In this seminar we will discuss QUT's H2Xport Project that is an ARENA funded project with University and Industry partners. The flagship activity in the project is a flexible, plug and play, 50kW pilot plant with, both CPV and SiPV solar technologies, and multiple technology types of batteries, fuel cells and electrolyzers. The ARENA H2Xport project includes research in water sustainability for the renewable hydrogen industry. A description of the pilot scale renewable hydrogen plant and research in water sustainability will be provided along with the learnings so far.

A proton flow reactor system for electrical energy storage and bulk export of hydrogen as hydrogenated carbon-based material

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The novel ‘proton flow reactor’ system for medium and grid-scale electrical energy storage, and for producing hydrogenated carbon(C)-based powder for bulk export, will be described. This system has been developed and patented at RMIT University in an R&D project funded by ARENA. The proton flow reactor employs electricity from renewables to charge a flowing ‘slurry electrode¹’ of C-particles with hydrogen. Hydrogen in the form of protons/hydronium is obtained by water splitting. Solid hydrogenated C-powder for storage and transport – and hence possible export – is generated by removing the liquid from the slurry. At the destination, this C-powder is reconverted into a slurry and passed through a similar reactor operating in ‘fuel-cell’ mode to re-generate electricity. This system will be a scaled-up form of RMIT’s novel proton battery – a reversible PEM fuel cell that reversibly stores protons in its solid electrode without forming hydrogen gas. The technical feasibility of a proton battery with an activated carbon electrode was proven by the RMIT team in 2018². The key components of the proton flow reactor system for much larger scale electrical energy storage than the proton battery – including the primary porous carbon materials selected, slurry formation, the charging reactor (‘electrolyser mode’), methods for drying the slurry, powder storage options, and the discharging reactor (‘fuel cell mode’) – will be described. Improvements in design and operation of these components achieved within the ARENA project will be reported, and the remaining technical challenges discussed.

References

¹ Mourshed, M., Niya, S.M.R., Ojha, R., Rosengarten, G., Andrews, J., Shabani, B., *Energy Storage Materials*, 2021, 40, 461-489.

² Heidari, S., Mohammadi, S.S., Oberoi, A.S., Andrews, J., *International Journal of Hydrogen Energy*, 2018, 43, 605-643

Reaction mechanism of proton storage in a proton flow reactor system: insights from DFT calculations

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The 'proton flow reactor' is a novel system for energy storage applications, developed and patented at RMIT University in an R&D project funded by the Australian Renewable Energy Agency (ARENA).^{1,2} The focus of this presentation will be on the use of density functional calculations and *ab initio* molecular dynamics (AIMD) simulations to ascertain the reaction mechanism of the proton storage process. Understanding such reactions is important for improving the composition of the electrode materials and for determining the storage mechanism of the reactor.³

In the proton flow reactor system, a carbon-based material is used to store the protons produced from hydronium ions in the flowing slurry electrode. The experimental results, specifically from XPS, Raman and IR measurements, indicate that oxygen is present on the carbon-based material, which may play a role in the proton storage process. In our DFT calculations and AIMD simulations, we model different types of surface bound oxygen and determine how they affect the adsorption of hydrogen on the surface. We compare this to the reaction that occurs on the surface in the absence of any adsorbed oxygen. We model the effect of reaction temperature and consider the effect of the charging and discharging processes on hydrogen storage. Overall, the calculations show that functionalised carbon-based material will readily store protons at temperatures of 0 K and above, through the formation of a surface-bound hydroxyl group. The results confirm the fundamental reactions that the proton flow reactor system rely upon are feasible.

References

¹ Mourshed, M., Niya, S.M.R., Ojha, R., Rosengarten, G., Andrews, J., Shabani, B., *Energy Storage Materials*, 2021, 40, 461-489.

² Heidari, S., Mohammadi, S.S., Oberoi, A.S., Andrews, J., *International Journal of Hydrogen Energy*, 2018, 43, 605-643.

³ Seif Mohammadi, S. Brennan, M. Oberoi, A., Vagh, H., Spencer, M.J.S., Dhilip Kumar, J. Andrews, J. *Energy Procedia* 2017, 110, 518.

Natural hydrogen seeps – implications for underground storage

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Natural hydrogen seeps called fairy circles have been identified in Mali, Brazil, Russia, and United-States (Zgonnik, V., 2020). Natural hydrogen is produced from a field in Mali for 7 years (Prinzhofer et al., 2018). The natural hydrogen system is still poorly understood and needs to be studied in new geological contexts such as the Precambrian cratons which appear very promising. In addition, the understanding of H₂ displacement and accumulation in subsurface and its interaction with the micro-organism will provide long-term constrains for underground storage numerical models.

In Australia, numerous circular surface features, commonly called salt lakes or swaps, are visible from the sky but no existing work shows nor quantifies any hydrogen content in those features. In this study, we reviewed the existing literature on fairy circles as to determine and directly test with soil-gas measurements if hydrogen surface-emitting features are present in Australia. We determined best candidates to test with a multidisciplinary approach linking geology, multi-physical imaging, and seismic interpretation.

Soil-gas measurements showed persistent hydrogen concentration localized in the external ring of circular depressions aligned along the Darling Fault (Figure 1, Frery et al. 2021), a major crustal boundary between the granitic, mafic and ultramafic rocks of the Yilgarn Craton from the sedimentary rocks of the Perth Basin. This work is the proof that fairy circles, in the meaning of H₂ emitting structures, are present in Australia and opens the door to a better understanding of the behaviour of underground H₂ at geological scale as well as new prospectivity pathways by evaluating original hypotheses on natural hydrogen generation, migration pathways and entrapment. This geological setting promotes deep serpentinization of ultramafic rocks as well as oxidation of iron-rich Archean rocks and mafic dikes as potential hydrogen sources that are of massive potential economic value. This hydrogen can circulate and be entrapped as aqueous hydrogen in low-salinity aquifers or migrate in gaseous phase in fault zones up to intermediate structural reservoir or to the surface.

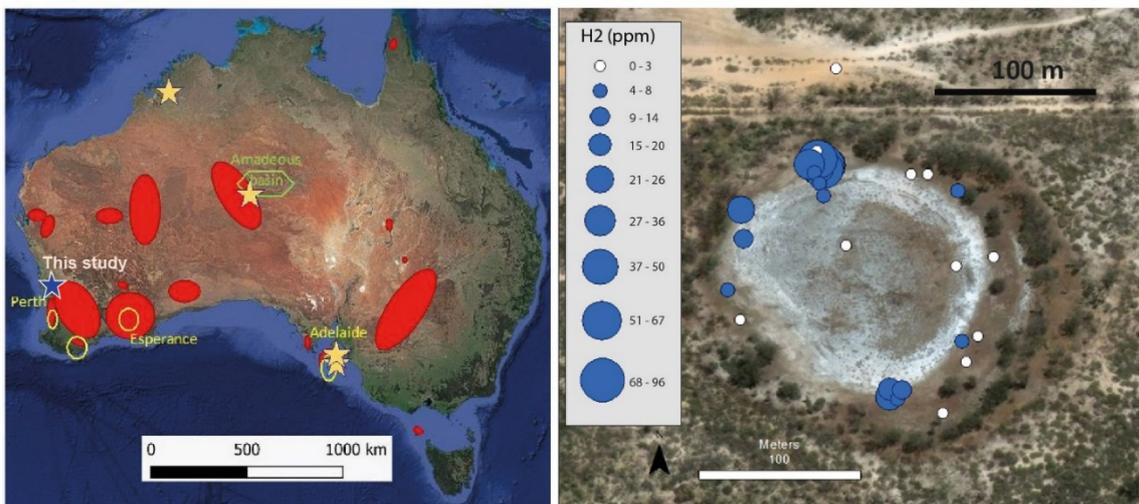


Figure 1. Natural Hydrogen seeps in Australia. Left: location of potential hydrogen seeps from a desktop study (Moretti et al., 2021). Right: First measurement of a circular Hydrogen seep in Australia (this study, Frery et al., 2021)

References

Frery, E., Langhi, L., Maison, M., & Moretti, I. (2021). Natural hydrogen seeps identified in the North Perth Basin, Western Australia. *International Journal of Hydrogen Energy*.

Moretti I, Brouilly E, Loiseau K, Prinzhofer A, Deville E. Hydrogen emanations in intracratonic areas: new guide lines for early exploration basin screening. *Geosciences* 2021a;11(x). <https://doi.org/10.3390/xxxxx>.

Prinzhofer A, Cissé CST, Diallo AB. Discovery of a large accumulation of natural hydrogen in Bourakebougou (Mali). *IJoHE* 2018;43(42):19315e26.

Zgonnik V. The occurrence and geoscience of natural hydrogen: a comprehensive review. *J Earth-Science Reviews* 2020:103140.

Green Electron Sessions

Hybrid Perovskite Quantum Dots for High Efficiency Solar Cells

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Perovskite quantum dots (QDs) have the advantages of quantum confinement effect, defect-tolerant nature, and the capability of developing lightweight and flexible films, thus attracting much recent research focus for a variety of functional device developments including QD solar cells. Here we report our recent progress on a new surface ligand engineering strategy in designing perovskite QDs, which led to a certified record power conversion efficiency of 16.6% in quantum dot solar cells. By using QDs as light absorbing materials, the QD based photocatalysts also exhibited good performance in photocatalytic gaseous hydrogen production.

Keywords: perovskites quantum dots, power conversion efficiency, water splitting

The multi efforts behind solar cell efficiencies: the fundamentals, characterisation and materials engineering

Hieu Nguyen, ANU

Over the past several decades, many research groups have been chasing efficiency records for solar cells. Moving towards higher efficiencies is the most direct way to reduce the cost of solar energy devices. However, behind each efficiency number are continuous advancements of many research areas, spanning the understanding of fundamental optoelectronic properties of materials, optimisation and development of new metrology techniques to monitor their evolutions and impacts on the device performance, and material engineering. In this talk, I will give updates on my team's recent advances in these areas, supporting the development of high-efficiency solar cells for both traditional and emerging technologies.

Design of Green Kesterite for Solar Photovoltaic and Photoelectrochemical CO₂ reduction

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Solar energy will be the renewable energy superpower, meeting the global energy needs while combating global warming challenges due its sustainability and carbon-neutrality. To capitalise this opportunity, equally sustainable energy materials is required for realising efficient energy conversion. Kesterite $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) is such an green energy material which is cheap, nontoxic, and chemically stable, with decent optoelectronic properties promising for solar photovoltaic and solar fuel applications. In recent years, there has been a significant research effort to develop CZTS-based devices focusing on discovering secret recipes that can solve the key obstacles to solar cell efficiency improvement, while branching out to other potential applications such as solar fuel. In this talk, our recent research progress on the design of kesterite-based devices will be reviewed, focusing on the defect engineering of kesterite for efficient solar-to-electricity generation, and as photocathode for photoelectrochemical CO₂ reduction.

Development of A PV/Thermal Solar Collector for Transforming Waste Sugar to Hydrogen

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Extracting hydrogen from biomass-derived alcohols (e.g., 5-hydroxymethylfurfural (5-HMF)) via solar-driven electrolysis represents a valuable approach by which a waste organic stream can be converted into hydrogen and other value-added chemicals ¹¹. Although significantly less energy (< ~30 kWh) is required to produce 1 kg of hydrogen using biomass-derived alcohols compared to water splitting ¹², a substantial amount *thermal* energy at medium temperature (up to 180 °C) is *also* required for pre-conditioning the biomass ¹¹. This dual energy need can potentially be provided via a hybrid PV-thermal collector. This approach represents an integrated, sustainable hydrogen production solution ¹¹. At present no viable design exists which can be mounted on rooftops, due to the need for tracking and relatively large space requirements. In this work, a ‘winged’ PV/T solar system (2.1 m² gross area) was designed and evaluated as a continuous power source (i.e., a maximum of ~300 W thermal and ~100 W of capacity) for transforming waste sugar to hydrogen. This design represents a new solar spectrum splitting method as sunlight can be selectively pre-absorbed by thin film PV cells (which are deposited onto a reflective metal foil substrate) for electricity, with the remaining spectrum (UV and IR) reflected and concentrated onto the thermal receiver/reactor. Theoretical and experimental analyses indicate that a thermal efficiency of up to ~25% can be achieved when operating at 150 °C ¹¹, while up to ~15% of PV efficiency ¹³ could be obtained from this PV/T collector. Furthermore, outdoor testing revealed that waste sugar was transformed directly inside the thermal receiver/reactor into bio-alcohols (i.e., 5-HMF) with a yield of up to ~20 mol %. The generated 5-HMF can be subsequently used to produce hydrogen in an electrolyser at a production rate of ~12 g per day per m² of solar collector gross area (under an average daily solar exposure of 5 kWh/m²). Overall, this study offers an efficient PV/T system (with an overall solar to hydrogen efficiency of 10-15%) which simultaneously up-grades abundant solar energy and waste biomass resources to value-added renewable hydrogen.

References

- [1] Li Q, Zhuo Y, Shanks K, Taylor RA, Conneely B, Tan A, et al. A winged solar biomass reactor for producing 5-hydroxymethylfurfural (5-HMF). *Solar Energy*. 2021;218:455-68.
- [2] Chen YX, Lavacchi A, Miller HA, Bevilacqua M, Filippi J, Innocenti M, et al. Nanotechnology makes biomass electrolysis more energy efficient than water electrolysis. *Nature Communications*. 2014;5:4036.
- [3] Jiang J, Giridharagopal R, Jedlicka E, Sun K, Yu S, Wu S, et al. Highly efficient copper-rich chalcopyrite solar cells from DMF molecular solution. *Nano Energy*. 2020;69:104438.

H₂ Transitions Sessions

What part can coal-derived hydrogen play in Australia's Energy Future?

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As we power towards a low carbon future, where could fossil fuels (coal and natural gas) fit into the equation? Is coal in a net zero world a possibility? Is it a means of kick-starting or scaling up the hydrogen economy in Australia and around the world?

This presentation will attempt to answer these questions.

Hydrogen Industry Progress Indicators: A Data Framework for Tracking the Hydrogen Value Chain

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The emergence of the hydrogen industry with its suite of technologies and applications is advancing at a rapid pace. In 2019 the Energy Council of the Council of Australian Governments (COAG) published the National Hydrogen Strategy the first national level strategy for the development of the clean hydrogen industry in Australia. Tracking and measuring its market signals that can quantify progress and identifying choke points in the industry's development is a priority for government and the hydrogen industry itself in order to give Australia a first mover advantage as an exporting nation. The National Strategy described 'progress indicator' areas, but measuring this progress and knowing whether Australia is on track to become 'a bulk export superpower' is a challenge in its own. In this research, a draft framework for tracking progress across hydrogen applications was developed based on the National Hydrogen Roadmap, is presented. In addition to presenting this framework, a number of insights to enhance robust and transparent assessments of the industry will be discussed. The research identified knowledge and research gaps, as well as options for further development of a tracking system and actions to be taken in the short-run and the long-run.

Delivering Hydrogen Transport Solutions Fit for the Future

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Ricardo will bring its worldwide experience with emerging technologies across the hydrogen value chain to the 4th Energy Future Conference. We have placed decarbonisation and sustainability at the heart of our strategy. We have an extensive range of skills relating to the hydrogen agenda, from policy development to infrastructure feasibility through to implementation and integration of hydrogen based technologies¹. Ricardo will present how we solve difficult engineering challenges in multiple transport applications and how this is shaping the future of the hydrogen energy ecosystem.

HYDROGEN FOR ROAD TRANSPORT

Hydrogen lends itself particularly well to heavy duty powertrain applications where heavy cargo or longer journeys are required. Ricardo has created a hydrogen-fuelled research engine which will offer a renewable, economic, and durable technology solution to accelerate zero carbon emissions in heavy duty trucks and off-highway machines.

HYDROGEN FOR RAIL

Ricardo has worked on hydrogen related projects in rail, including Porterbrook's HydroFLEX, the first hydrogen-powered train to operate in the UK, whilst a project in the Netherlands for the province of Groningen assessed the viability of hydrogen fuel cell range-extended battery-powered trains.

HYDROGEN FOR MARINE

Hydrogen will play a critical role in enabling the marine industry to meet its targets of significantly reducing carbon emissions and limiting its impact on climate change. Ricardo's alternative fuel and renewable energy experts have been supporting the industry, operators, and ports with understanding the policies and technologies needed to support achievement of mandatory emission requirements.

HYDROGEN FOR AEROSPACE

Project Fresson will deliver an emissions-free, hydrogen-fuel-cell-powered flying demonstrator by September 2022. Having completed a comprehensive evaluation of technologies and configurations for sustainable aircraft propulsion, the Fresson team concluded that hydrogen fuel cell technology is the optimum solution to meet environmental, regulatory, and operational requirements for this size of aircraft, enabling zero carbon emissions and reducing operating costs.

Reference

1. Ricardo.com. (n.d.). Hydrogen for Transport. [online] Available at: <https://ricardo.com/hydrogen> [Accessed 30 Aug. 2021].

Public Perceptions Towards Hydrogen Energy Technologies Across the Value Chain

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The successful development of any new energy technology is dependent on public acceptance¹. Past research suggests that people, even though they have low awareness, are generally supportive of some types of Hydrogen Energy Technology (HET)². Namely, hydrogen fuel cell vehicles and hydrogen fuelling stations. However, few studies have investigated how people think about other types of HET³. Considering hydrogen can be made, stored, moved and used in different ways, public support is likely dependent on people's perceptions towards specific types of HET. This presentation will highlight the findings from a recent study exploring people's beliefs about, and support for, HET across the hydrogen value chain.

To understand how people think about different types of HET, a qualitative study involving thirty metropolitan residents who participated in four focus group sessions was undertaken in May 2021. Because most people have low knowledge about HET^{2,4}, participants were provided with information about various types of HET, which highlighted the expected risks, benefits and costs associated with the different technologies⁵. Two short surveys were also used to assess the impact of information provision on participants' subjective knowledge and support for HET.

The findings suggest that people's support for HET is, to some extent, dependent on production and application approaches. Some participants, for instance, believed that hydrogen energy had limited utility for household heating applications due to the perceived risks and costs. Others expressed concerns about producing hydrogen with Carbon Capture and Storage technology and storing hydrogen underground due to the perceived environmental impact and leakage risk. There was, though, generally a positive attitude towards hydrogen as a future energy carrier, and support for further research, development and pilot projects. The results highlight the importance of a technology-specific approach to public engagement to meet community expectations, and to ensure public support and a social licence to operate.

References

- ¹Wüstenhagen, R., Wolsink, M., & Bürer, M. J. (2007). Social acceptance of renewable energy innovation: An introduction to the concept. *Energy Policy*, 35(5), 2683–2691. <https://doi.org/10.1016/j.enpol.2006.12.001>
- ²Ricci, M., Bellaby, P., & Flynn, R. (2008). What do we know about public perceptions and acceptance of hydrogen? A critical review and new case study evidence. *International Journal of Hydrogen Energy*, 33(21), 5868–5880. <https://doi.org/10.1016/j.ijhydene.2008.07.106>
- ³Emodi, N. V., Lovell, H., Levitt, C., & Franklin, E. (2021). A systematic literature review of societal acceptance and stakeholders' perception of hydrogen technologies. *International Journal of Hydrogen Energy*. <https://doi.org/10.1016/J.IJHYDENE.2021.06.212>

POSTERS

Presentation

Experimental Study on the Effect of Adding Hydrogen on the Combustion Characteristics of Methane in Small space

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Micro power system has been widely used in many fields of production and life. As the core component of micro-power systems, the combustion stability of micro-burners has attracted extensive attention. Studies have shown that adding hydrogen can improve the flame stability under small-scale combustion. An experimental platform was built in this study and it was concluded that the methane flame would show three states of "stable flame", "FREI flame" and "quenching" as the combustion space reducing. In the stable flame range, the flame front temperature decreases as the space decreases, and the flame front temperature increases with a larger excess air coefficient at the same space. It shows that the addition of hydrogen will widen the combustion scale limit, so that the flame can burn stably at a space of 5 mm. The "FREI flame" period of methane becomes smaller and the maximum velocity becomes larger after adding hydrogen, while the peak velocity is reached sooner. In addition, hydrogen addition increases the range of stable flame interval and decreases the range of "quenching" interval, which effectively broadens the combustibility range of the flame.

Effect of Adding Hydrogen on the Concentration of Gaseous Group in Diamond Prepared by Combustion Flame Method

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The generation of natural diamond requires harsh high temperature and high-pressure environment, so its storage is very small in nature. Diamond could be synthesized by combustion of C₂H₂ with a certain gas ratio in O₂. In this paper, the chemical reaction process of synthetic diamond by combustion flame method is studied. The influence of different amount of hydrogen on the active group in acetylene flame was elucidated. By importing Chemkin acetylene detailed reaction mechanism, the temperature field of acetylene flame and the concentration distribution of important groups such as H, OH and HCCO in the flame were analyzed after adding hydrogen at different flow rates of 0L/min, 0.1L/min, 0.2L/min, 0.3L/min, 0.4L/min and 0.5L/min. Addition of hydrogen could increase the concentration of H group, HCCO group and OH group in the flame without changing the flow rate of oxygen and acetylene, which is beneficial to the nucleation and growth of diamond.

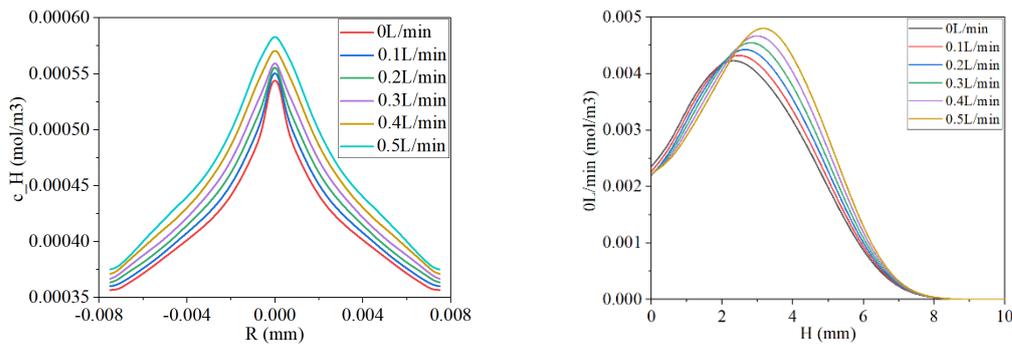
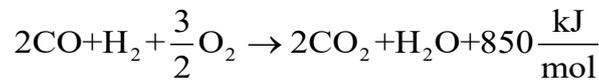


Figure 1. Radial distribution curve of H atom concentration (left). Axial distribution curve of HCCO group concentration (right)

References

- [1] L Huang, T Wang, Y Tang. Integration Technology, 04, (2017), 72-81.
- [2] Y Hirose. Journal of the Japan Society for Precision Engineering, 53, (1987), 51-56.
- [3] Z Guo. Chinese Journal, 36, (1991), 638-639.
- [4] R.J.H. Klein-Douwel, J.J. Meulen, Journal of Applied Physics, 33, (1998), 13-21.
- [5] L Wen, Y Xia, Y Mo, et al. Journal of Inorganic Materials, 12, (1997), 613-616.

One step synthesis of molybdenum carbide nanoparticles for efficient hydrogen evolution reaction

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Hydrogen has been promoted as an alternative source of energy, which is renewable, cost-effective and nature friendly. Hydrogen evolution reaction (HER) can be used for mass production of hydrogen at a very low cost through electrochemical water splitting. An active and efficient electrocatalyst is required to perform this reaction. Till date, platinum (Pt) is a stable and efficient electrocatalyst towards her. But its high cost and low abundance hinders its large scale uses. Molybdenum carbide having a similar electronic structure to platinum can be a great alternative to costly platinum. In this study, pure phase molybdenum carbide (Mo_2C) has been synthesized in a single step. Synthesis temperature and holding time has been optimized to obtain pure phases of mo_2c . The surface, structural and morphological properties of as-synthesized compounds has been studied. The HER activity of as-synthesized compounds has been explored in detail.

Hydrogen Generation Potential from Biogenic Residues of Bangladesh

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The rapid depletion of fossil fuels and the impending consequences of global warming led the movement to transitioning towards cleaner pathways for energy production. One of the most promising candidates for a clean and universal energy carrier is hydrogen. At present, 95% of hydrogen is produced from fossil fuel while only 5% is generated from renewable resources. Developed countries have been rapidly facilitating third-generation technologies for sustainable hydrogen production. However, developing countries are yet to be included in the global H₂ economy transition. Bangladesh, a low-income country, is not only rapidly running out of its fossil fuel reserves, but also at the forefront of facing adverse effect of global climate change. Studies estimate that Bangladesh will likely run out of indigenous fossil reserves by 2050 and face an energy resource vacuum, risking its economy. However, being a densely populated and agriculture-focused country, Bangladesh has immense biomass waste in the form of biogenic residues, such as agricultural waste, dairy farm, etc. According a 2020 report by World Bank, the per capita GHG emission in Bangladesh increased by more than 45% from 2010 to 2020, attributed to fossil fuel usage and disposal of biogenic waste. More than 60 million tons of biogenic waste are generated in the country, which includes livestock waste, field and crop-based residues. which possess an enormous potential to be utilized for sustainable H₂ production. A preliminary estimation indicates that approximately 2 million tons H₂ can be produced annually by utilizing current biogenic waste. This submission focuses on the H₂ generation potential of biogenic residues generated by Bangladesh; namely the potential of switching to H₂ economy utilizing biogenic waste in the context of the country's present infrastructure.

Hydrogen generation through banded iron formation (BIF) oxidation: a new resource for Australia?

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The oxidation of iron rich rock can generate H₂ in oceanic as well as in continental domains. Here we tested the potential for Banded Iron Formations (BIF), Precambrian iron-rich sedimentary rocks, to produce H₂ during weathering. The potential of these rocks for H₂ generation is very high, as they account for more than 60% of world global iron reserves with low Fe³⁺/Fe-total before weathering. In addition, satellite imagery in Australia and Brazil revealed the presence of sub-circular depressions, that usually are the proxy of H₂-emitting features (Moretti et al., 2021), in the vicinity of iron mines hosted in BIF.

A petrological study conducted on fresh and weathered BIF samples from the Hamersley Province in Western Australia, shows that the weathering of the BIF has the potential to produce H₂ by oxidation under surface conditions. The mineralogical study shows transitions from stilpnomelane (a ferrous silicate) and ankerite (a ferrous carbonate) to goethite (FeOOH) and from magnetite (FeO Fe₂O₃) to maghemite (γ -Fe₂O₃), hematite (α -Fe₂O₃) and goethite. The oxidation of ferrous iron from BIF by low temperature aqueous fluid is a promising mechanism for potential hydrogen production. The BIF weathering mineralogy suggests that low temperature aqueous fluids have the potential to generate H₂, challenging the idea that high temperature is always required to generate hydrogen as it is the case during serpentinisation. This new source of hydrogen could enhance Australia natural H₂ potential in addition to the radiolysis quantified by Boreham and al (2021) or to water reduction (Frery et al., 2021).

Decarbonization through Conversion of CO₂ and Renewable Energy to Chemicals Fuels via Synthesis Gas

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The success of global efforts to achieve net-zero CO₂ emissions is contingent on cost-effective methods of closing the carbon loop. Utilizing renewable energy to drive the electrochemical reduction of CO₂ (CO₂RR) to value-added chemicals (i.e. renewable Power-to-X) offers the dual advantage of converting intermittent renewable energy to a stable chemical form, whilst simultaneously reducing the emission of waste CO₂ to the atmosphere.^{1,2}

A highly favourable product of CO₂RR is synthesis gas (or syngas), generated by the conversion of CO₂ and water (present in the humidified CO₂ inlet stream) to CO and H₂. Syngas is a key building block for the production of a wide range of chemicals, including synthetic liquid fuels such as ethanol and methanol, and plastic packaging materials.³ The syngas and derivatives market is projected to grow significantly (over 6% p.a.) over the next decade, driven by increased demand for syngas derivatives, as well as a global push for more environmentally-friendly sources of energy and products.^{4,5}

My research focuses on designing both nanomaterials and electrochemical systems for the application of CO₂RR to syngas on a commercial scale. Catalyst engineering on a nano scale involves the creation, tuning, and manipulation of active sites within a catalyst structure, promoting high activity towards a desired syngas ratio (H₂:CO ratio). Furthermore, our catalysts are developed using low-cost and scalable materials and synthesis approaches, as well as exhibiting tolerance to input stream impurities. We also focus on macroscale electrode engineering, involving fabrication of gas diffusion electrodes exhibiting specialised components, devoted to charge transfer, liquid inhibition, vapour transport, and catalyst bonding. Finally, we look at the overall system development and optimisation at a large scale, including a cell setup capable of continuous, vapour-fed CO₂RR, as well as investigating reduction of operational expenditure, through methods such as application of waste heat to increase production rate.

References

1. Shih CF, Zhang T, Li J, Bai C. Powering the Future with Liquid Sunshine. *Joule*. 2018;2(10):1925-1949. doi:10.1016/j.joule.2018.08.016
2. Daiyan R, MacGill I, Amal R. Opportunities and Challenges for Renewable Power-to-X. *ACS Energy Lett*. Published online November 15, 2020:3843-3847. doi:10.1021/acscenergylett.0c02249
3. Wender I. Synthesis gas as a source of fuels and chemicals: C-1 chemistry. *Annu Rev Energy*. 1986;11:295-314. doi:10.1146/annurev.eg.11.110186.001455
4. Market Research Engine. Syngas Chemicals Market Research Report. Published 2020. Accessed October 22, 2020. <https://www.marketresearchengine.com/syngas-chemicals-market>
5. Syngas & Derivatives Market by Production Technology, Gasifier Type, Feedstock (Coal, Natural Gas, Petroleum Byproducts, Biomass/Waste), Application (Chemicals, Fuel, and Electricity), and Region - Global Forecast to 2025. Accessed September 28, 2020. <https://www.marketsandmarkets.com/Market-Reports/syngas-market-1178.html>

Underground Hydrogen Storage: fundamental studies on hydrogen wettability

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Underground Hydrogen Storage (UHS) is considered a long-term storage solution which allows excess energy developed from renewable energy sources to be stored in form of hydrogen in the subsurface reservoirs and retrieved when energy demand increases. Research into UHS has been increasing in recent years, with a focus on determining the petrophysical properties of hydrogen interacting with fluid and subsurface rocks. UHS in porous media targets depleted gas reservoirs and aquifers. The focus of this work is to determine the wettability and Interfacial Tension (IFT) of the hydrogen-brine-quartz system using different methods for wettability, the captive bubble method and in-situ analysis using 3D micro-Computed Tomography (CT) imaging, and the pendant drop method for IFT. The captive bubble method provides the intrinsic contact angle which remained in the range 29-39° for pressures 1000-3000 psi and salinities from distilled water to 5000ppm NaCl brine. The in-situ method determines the macroscopic contact angle and contact angle distribution.

The mean value of contact angle is 59.75°. The IFT is found to decrease with increasing pressure in distilled water from 72.45 mN/m at 1000 psi to 69.43 mN/m at 3000 psi. No correlation was found between IFT and salinity for the 1000ppm and 5000ppm brine. Our fundamental studies provide insights into physics of hydrogen displacement in the multiphase environments of subsurface reservoirs and can be used for modelling storage capacity and withdrawal rate of hydrogen.

Transformation of Waste NO_x to Ammonia

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The clean sole combustion product of H₂ – water only, has caused H₂ to emerge as a critical vector for green energy future in replacement of current fossil fuels. However, the application of H₂ as a fuel and/or energy carriers is still vastly limited by its transportation and storage issue due to its high flammability and gaseous properties under ambient conditions.^{1,2} To tackle this, NH₃ has been suggested as one of the most promising energy carriers for H₂ owing to its liquid properties at room temperature and 10 bar, as well as greater hydrogen content compared to H₂ itself.² Moreover, the readily available regulations and infrastructure for NH₃ handling and transportation aids the facilitation of global hydrogen economy^{2,3} (also referred as Hydrogen 2.0⁴). Nevertheless, NH₃ today is still mainly manufactured by the non-environmentally friendly and energy intensive Haber Bosch process which utilizes fossil fuels as H₂ feedstock and has contributed significantly to global greenhouse gases emission.⁵

Therefore, herein, the reported finding is to use plasma-electrolyser hybrid system to convert air and water into intermediary NO_x, and subsequently being synthesized into NH₃.⁶ This approach provides an opportunity for complete green energy cycle and decentralized local production. The generated NH₃ can be readily used as H₂ fuel via NH₃ splitting or feedstock in industry. Furthermore, it also provides economic opportunity by treating NO_x from powerplants, industries and agricultural waste as resources rather than unwanted emissions.⁴ As such, it is critical to develop simple and inexpensive catalysts for effective conversion of NO_x into NH₃. Our research is focused on reducing the levelized cost of NH₃ by lowering cell potential and improving process current density.⁴ The ultimate goal is to meet an NH₃ production of 600 g/m²/h (by CSIRO) to initiate Hydrogen 2.0.¹ To this end, we developed CuO_x/Cu foam catalyst via electrodeposition and demonstrated relatively high NH₃ production rate (42.5 nmols⁻¹cm⁻²) and Faradaic efficiency (85%) at -0.5 V_{RHE}, exhibiting large attainable NH₃ yield at fairly low applied potential.

References

- (1) Bruce, S.; Temminghoff, M.; Hayward, J.; Schmidt, E.; Munnings, C.; Palfreyman, D.; Hartley, P. *National Hydrogen Roadmap*; Australia, 2018.
- (2) Giddey, S.; Badwal, S. P. S.; Munnings, C.; Dolan, M. Ammonia as a Renewable Energy Transportation Media. *ACS Sustain. Chem. Eng.* 2017, 5 (11), 10231–10239.
- (3) Cheddie, D. Ammonia as a Hydrogen Source for Fuel Cells: A Review. In *Hydrogen Energy: Challenges and Perspectives*; InTech, 2012; pp 333–361.
- (4) Daiyan, R.; Tran-Phu, T.; Kumar, P.; Iputera, K.; Tong, Z.; Leverett, J.; Khan, M. H. A.; Asghar Esmailpour, A.; Jalili, A.; Lim, M.; Tricoli, A.; Liu, R.-S.; Lu, X.; Lovell, E.; Amal, R. *Energy Environ. Sci.* 2021, 14 (6), 3588–3598.
- (5) Carreon, M. L. Plasma Catalytic Ammonia Synthesis: State of the Art and Future Directions. *Journal of Physics D: Applied Physics*. IOP Publishing 2019.
- (6) Sun, J.; Alam, D.; Daiyan, R.; Masood, H.; Zhang, T.; Zhou, R.; Cullen, P. J.; Lovell, E. C.; Jalili, A.; Amal, R. A Hybrid Plasma Electrocatalytic Process for Sustainable Ammonia Production. *Energy Environ. Sci.* 2021, 14 (2), 865–872.

Disordered perovskite-type oxides using biomineralisation approach for H₂ related applications

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The world is shifting towards developing a hydrogen (H₂) economy to reduce the use of fossil fuel and escalating CO₂ emissions. Biological system has provided us inspirations to design and engineering new catalyst for green H₂ production. For example, microorganisms use proteins to make inorganic structures in an environmentally friendly process termed biomineralization. Compared to conventional synthesis, biomineralization approach can offer the capacity to make material with disordered structure, particularly wherein access to disordered surface structure is beneficial. This material could exhibit better catalytic performance for a variety of functional applications, such as Ti_aZr_bO_x for HMF production which can be subsequently convert to H₂, or Sn_aZn_bO_y for H₂ production as a by-product under CO₂ reduction reaction. Controllable bimetallic ratio could be achieved to modulate the surface active sites and material structures for performance optimisation. All materials are characterised using synchrotron characterisation to establish a relationship between the performance/selectivity and the material electronic/local structure. Through these efforts, we have demonstrated that biomineralization brings a new strategy to synthesis oxide-based catalyst for H₂ related applications.

Atomic Co decorated free-standing graphene electrode assembly for efficient hydrogen peroxide production in acid

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The past fifty years have seen a strong interest in the electrosynthesis of acidic hydrogen peroxide (H_2O_2) via oxygen reduction reaction (ORR) in both academia and industry because its advance can drastically benefit downstream environmental treatments.¹⁴ However, up to now, the apparent activity of most electrocatalysts (especially in a flow cell reactor) still calls for improvement to meet the industrial demands which require a stably high H_2O_2 productivity with low energy input. In this talk, we will present a fresh free-standing ORR electrode design to achieve energy-efficient acidic H_2O_2 synthesis with a high production rate. This electrode comprises cobalt single atoms on vertically aligned graphene nanosheet assembly (CoN_4/VG), which exhibits a hierarchical porous structure that can maximize the utilization of catalytic active atoms without sacrificing the mass/charge transport efficiencies. Therefore, it can give a H_2O_2 selectivity close to 100% from 0.3 to 0.5 V versus reversible hydrogen electrode (RHE) in 0.1 M HClO_4 within H-cell setup, and sustain a record-breaking high H_2O_2 productivity of $706 \text{ mmol}_{\text{H}_2\text{O}_2} \text{ g}_{\text{catalyst}}^{-1} \text{ h}^{-1}$ at 0.3 V vs. RHE for 36 hours. When this electrode is introduced into an industrially relevant flow reactor, more promisingly, it can allow a peroxide concentration of 1100 mg L^{-1} ($4000 \text{ mmol}_{\text{H}_2\text{O}_2} \text{ g}_{\text{catalyst}}^{-1} \text{ h}^{-1}$) continuously at -1.8 V of cell voltage corresponding to the energy consumption of $3.81 \text{ Wh g}_{\text{H}_2\text{O}_2}^{-1}$, which represents the most energy-efficient flow system for rapid H_2O_2 generation in acidic media.

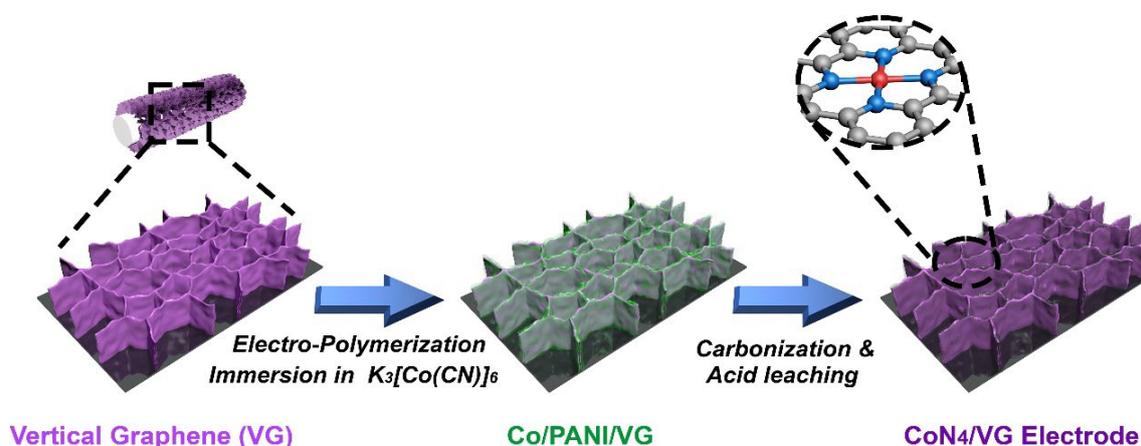


Figure 1. Electrode design for efficient hydrogen production in acid

References

¹ Brillas, E. *Chemical reviews* 2009, 109 (12), 6570-6631.

Numerical study of 5-hydroxymethylfurfural production in an innovative winged solar biomass reactor

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5-Hydroxymethylfurfural, as a biomass-derived alcohol, is a promising intermediate for value-added chemicals and hydrogen production (electrolysis). To produce this valuable product in an environmentally friendly way and minimise its energy consumption, an innovative winged solar-driven biomass reactor is built. This reactor combines the concept of the solar concentrator and phase-change material to efficiently utilise and store the solar energy for hydrolysis reaction requirements. A transient computational fluid dynamics model is developed to describe the energy transfer during the phase change material liquidation and solidification along with the daily solar radiation. Also, the heat and mass transfer phenomena during the 5-Hydroxymethylfurfural production are illustrated. This numerical model is validated against the experimental measurements, and it is employed to numerically evaluate the reactor's performance under different operating schemes. The simulation results indicate that the amount and type of the charged phase change materials affect the yield of 5-Hydroxymethylfurfural and the by-products due to the heat storage capacity. In addition, the heat absorption and desorption of the phase change material make the inner tube reactor maintain a mild heating environment and extend the reaction time, which improves the system efficiency. This model provides a cost-effective way to understand and optimise the solar-driven reactors.

Keywords: Phase change material, Solar-driven reactor, CFD, Numerical modelling

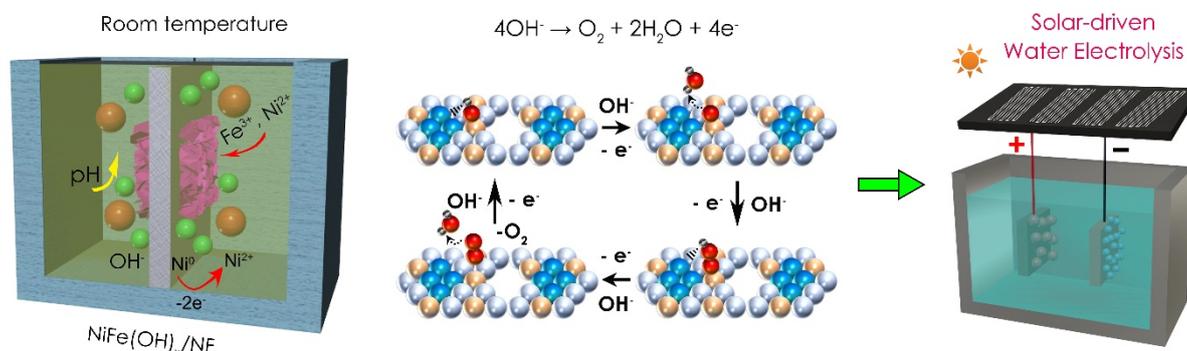
Room-Temperature Synthesis of Defect-Rich, Ultrathin Nickel-Iron Hydroxides with High Overall Water Splitting Activity

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The production of hydrogen via alkaline water electrolysis powered by the solar-generated renewable electricity has received great attention over the past decade as it offers an efficient means to locally convert the intermittent solar energy to clean chemical fuels.^{1,2} A high-performance alkali electrolyser requires highly active and stable anode and cathode.³ Low-cost construction of electrocatalysts with high activity and long cycling life plays a crucial role in electrocatalytic water splitting. Here, we report a facile room-temperature one-step strategy for in-situ growth of defect-rich ultrathin nickel-iron hydroxides (NiFe(OH)_x) nanosheets on Ni foam (NF), realized by simply immersing NF in an extremely small volume of mixed nickel-iron (Ni-Fe) nitrate aqueous solution. The prepared NiFe(OH)_x/NF electrodes exhibit remarkable activity towards both oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), and can afford high current densities up to 1 A cm⁻². A two-electrode overall water splitting device is assembled using NiFe(OH)_x/NF as both the anode and cathode, which achieves 10 mA cm⁻² at 1.50 V in 1 M KOH when powered by a commercial silicon solar cell.



References

- [1] J. Luo, J.-H. Im, M. T. Mayer, M. Schreier, M. K. Nazeeruddin, N.-G. Park, S. D. Tilley, H. J. Fan and M. Grätzel, *Science*, 2014, **345**, 1593-1596.
- [2] M. F. Lagadec and A. Grimaud, *Nat. Mater.*, 2020, **19**, 1140-1150.
- [3] Y. P. Zhu, C. Guo, Y. Zheng and S. Z. Qiao, *Acc. Chem. Res.*, 2017, **50**, 915-923.

Low Temperature Photo enhanced CO₂ Reduction to CH₄ using Co- La/TiO₂ Catalysts

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The conversion of CO₂, a major constituent of greenhouse gases, to valuable fuels by sunlight is of significant interest due to the potential of using both light and heat from the sun to invoke sustainability in conventional energy-consuming chemical reactions.¹ In this study, with the intent of reducing thermal energy requirements as well as understanding the potential for light enhancement, the impact of visible light illumination on Co-La catalysts (loaded on TiO₂) for the CO₂ methanation reaction was examined. Specifically, Co with different La loadings on a TiO₂ support was exposed to white LED illumination under reaction conditions and the effect on catalyst activity and selectivity was investigated. In most cases light illumination delivered better catalytic activity over the temperature range 250- 450°C. Of particular interest was the change in catalytic properties with the addition of La on TiO₂ support. In the case of Co₁₀-La₁₀/TiO₂, white light illumination ($\lambda = 300-780$ nm) lowered the activation energy by 20% and facilitated an 86% enhancement in CO₂ conversion (from 10% to 19% CO₂ conversion at 350°C). With different characterisations, it was revealed La promotion has potential to decrease crystallite size of Co, improved surface basicity and create more oxygen vacancies on the TiO₂ surface. Further detailed investigations with In-situ characterisations demonstrated the basic sites introduced by La played a pivotal role in enhancing CO₂ adsorption and its transformation to an intermediate specie susceptible to light enhancement. The absence of significant light enhancement on sample without La addition (Co₁₀/TiO₂) further validated the importance of La addition in this work and confirmed the observed light enhancement on La based samples was not invoked by photothermal heating.

Proposed hydrogen production, distribution, and export facility within the Port Botany and Kurnell precincts, NSW, Australia

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This poster presentation considers a proposed hydrogen production, distribution, and export facility within the Port of Botany, and Kurnell precincts in NSW, Australia.

It will evaluate the production, distribution, and export of hydrogen in the form of ammonia; dimethyl ether [DME]; methanol; and/or liquid organic hydrogen carriers [LOHC], thereby transforming existing under-utilized infrastructure that may be combined for another use.

This may be achieved through proposed modifications to existing water treatment infrastructure at the Sydney Desalination plant, and land within the former Ampol lubricating oil refinery precinct, by employing renewable energy generated at the Woodlawn Capital Renewable Energy wind farm that might be converted into hydrogen, and/or other energy carriers within the former refinery precinct.

Correspondingly, this research considers the deployment of a fleet of hydrogen vehicles as part of a metropolitan hydrogen network, the: processing; freight; and conversion of municipal waste into bioenergy; and the adoption of a circular economy methodology to the local hydrogen industry.

In doing so the author will evaluate how existing liquid fuels infrastructure might be accessed thereby responding to the opportunity, but also how existing petroleum, and waste disposal industries might be transformed through the production of molecules, rather than electrons.

Finally, this presentation considers the proposed export of the energy carrier from existing facilities in New South Wales thereby drawing inspiration from the:

Energy Park Mainz facility, Mainz, Germany; the George Olah Renewable Methanol plant, Svartsengi, Iceland; the H2Ocean project, European Union; Porsche / Siemens Energy - Hari Oni, Chile; the Raffinerie Heide conversion project, Schleswig-Holstein, Germany; the RH2INE Initiative, Zuid Holland, the Netherlands; and the Chiyoda Corporation SPERA project Sungai Liang Industrial Park, Brunei Darussalam.



Figure 1. Sydney Desalination plant, and former Caltex Kurnell oil refinery, Joseph Banks Drive, Kurnell [Sydney Desalination Plant, 2018]

Evaluation of Hydrogen Photocatalytic Production Parameters using TiO₂ doped with platinum under low-intensity radiation

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The energy issue is essential to ensure human development in the next generations, in recent decades the exponential loss of fossil fuel reserves due to overexploitation, aggravating subsequent pollution and accelerating global warming.¹ Which makes it essential to find a balance between energy development and the environment. Hydrogen (H₂) is a promising fuel, which is carbon-free and has a high energy density, and has been increasingly focused on investments.² In this context, heterogeneous photocatalysis emerges as one of the most promising ways of harnessing solar energy in the form of usable chemical energy. However, the influence of reactional parameters requires deeping analysis for large-scale feasibility.³ In this study, the glycerol photoreforming in aqueous medium was carried out through the activation of titanium dioxide doped with platinum (TiO₂@Pt), using a halogen lamp as a radiant source. A two-level (2k) factorial experimental design was carried out to evaluate the variables pH, glycerol concentration, photocatalyst concentration, and photodeposited platinum concentration on the TiO₂ surface. The response surface methodology (RSM) was used to indicate the condition of highest photocatalytic performance, obtaining a hydrogen production rate (HPR) of 1005.63 μmol H₂.g⁻¹.h⁻¹ with catalyst, platinum, and glycerol concentrations in 0.1 g.L⁻¹, 1.0% (w/w), 5% (v/v), respectively, and pH = 2. Additionally, the catalyst concentration was the only significant variable of the process, showing a negative correlation, that is, the lower concentration, the greater the response in terms of HPR.

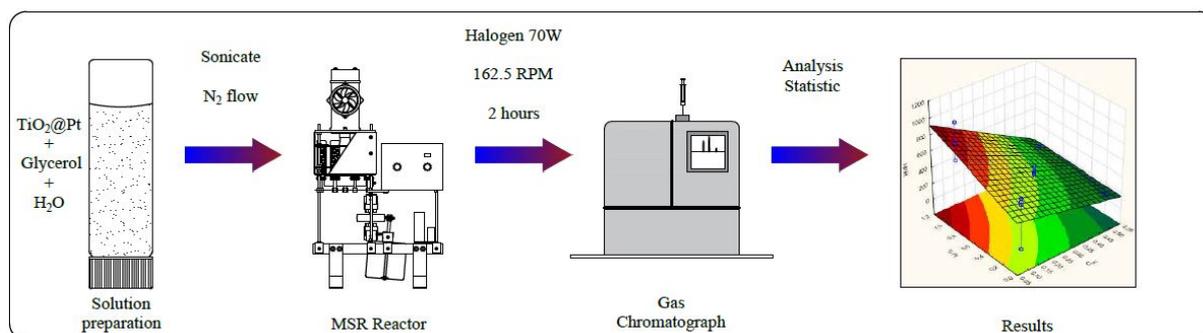


Figure 1. Illustration of the experimental process

Reference

- ¹ Ahmad, K.; Ghatak, H. R.; Ahuja, S. M. *Environ. Technol. Innov.* **2020**, *19*, 100893.
- ² Yu, S.; Han, B.; Lou, Y.; Liu, Z.; Qian, G.; Wang, Z. *Int. J. Hydrogen Energy* **2020**, *45* (53), 28640–28650.
- ³ Zhang, J.; Hu, W.; Cao, S.; Piao, L. *Nano Res.* **2020**, *13* (9), 2313–2322

Photocatalytic hydrogen production using Pt/TiO₂ as catalyst

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Techniques aimed at the production of hydrogen gas (H₂) are increasingly encouraged, especially in the field of renewable energies and in the field of green chemistry¹. In this work, the TiO₂/Pt photocatalyst was produced using the platinum photodeposition method on commercial titanium dioxide (P25, Degussa). The photocatalytic activities of this catalyst were tested in the hydrogen production with the presence of different alcohols as sacrificial agents: methanol, ethylene glycol and glycerol. Xenon lamp was used as a light source. The hydrogen production was analyzed in 6 hours of reaction, in an alcoholic solution of 3% and catalyst concentration of 0.5 g.L⁻¹. The best result was obtained using glycerol as a sacrificial reagent at the concentration, producing a rate of 2510 μmol.h⁻¹.g⁻¹. In terms of hydrogen production, the ordering of the sacrificial agents was: glycerol > ethylene glycol > methanol. Furthermore, different percentages of platinum were tested (0.1, 0.27, 0.45 and 0.57%), in which the H₂ production rate (HPR) was higher using 0.1% of platinum. Using glycerol as substrate and Pt/TiO₂ (0.1%) as catalyst, the rate of hydrogen production kinetic was quantified. It is possible to observe that in 3,5 hours of reaction the HPR stabilizes. Furthermore, its photonic efficiency was determined using the actinometric method, reaching 0.42%.

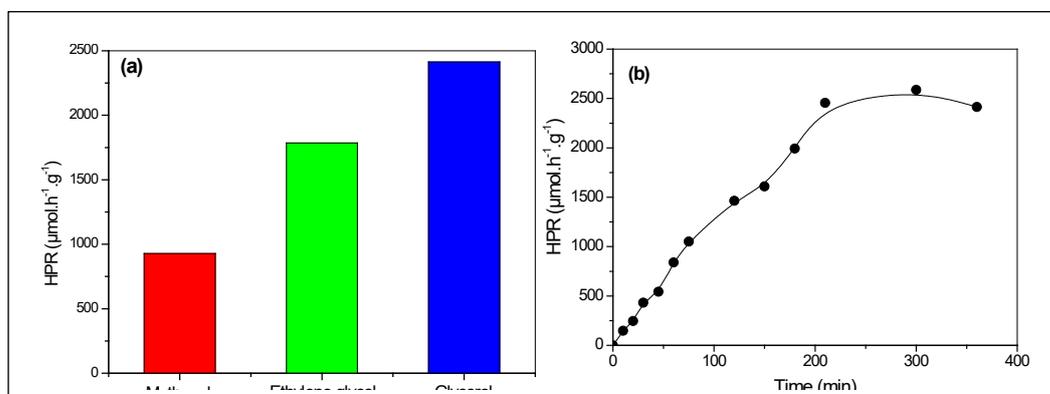


Figure 1. Hydrogen Production Rate: study of different alcohols as sacrificial agentes (a), and glycerol photoreforming kinetics (b). $C_{\text{glycerol}} = 3\%$, $\text{TiO}_2/\text{Pt} (0.1\%) = 0.5 \text{ g.L}^{-1}$.

Reference

¹PUGA, A. V. Photocatalytic production of hydrogen from biomass-derived feedstocks. *Coordination Chemistry Reviews*, v. 315, p. 1–66, 2016.

Recycling of components of wasted solid oxide electrolyzers or fuel cells

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Summary: Decarbonized hydrogen production is expected to play a key role in the transition to a sustainable fossil free economy ¹. However, high demand for carbon free hydrogen requires large size Solid Oxide Electrolyzers (SOEs) which in turn have economic, environmental and legislative problems of end of life products ². To solve this problem, we are attempting a strategy to recycle and reuse Solid Oxide Cells (SOCs) components and regenerate electrolytes. The separation of electrode-electrolyte assembly was performed through mechanical scratching and grinding followed by thermal and chemical treatments. Recycle materials of SOFCs components; air electrodes ($\text{La}_x\text{Sr}_{1-x}\text{CoO}_3$), nickel oxide (NiO) which constitutes about 50% in weight of the cell and Yttria Stabilized Zirconia (YSZ) were successfully obtained. Detailed crystallographic studies, microstructure, and compositions of the recovered materials were studied respectively by X-Ray Diffraction and Scanning Electron Microscope/Energy Dispersive X-Ray Spectroscopy. The electrical conductivity of the recycled electrolyte pellets was measured in air by Electrochemical Impedance Spectroscopy from 250 °C to 715 °C. The conductivity of the electrolyte made from recycled materials of SOC wastes was compared with different composition of commercial YSZ materials ³⁻⁵. A total electrolyte conductivity of $4.8 \times 10^{-3} \text{ S cm}^{-1}$ was measured at 700 °C. The lower level of conductivity of the regenerated electrolyte material is discussed and improvements to increase it are suggested.

Reference

- 1 Hosseini, S.E., Wahid, M.A., *Renew. Sustain. Energy Rev*, **2016**, vol 57, 850-866
- 2 Wright, E.I, Clegg A. J and Rahimifard S., J., *Power Sources*, **2009**, vol 190, 362-371
- 3 Mæland, D, Suci, C., Waernhus, I., Hoffmann, A.C., *Eur. Ceram*, **2009**, vol. 29, pp. 2537-2547
- 4 Zhang, J., Lenser, C., Menzler, N.H., Guillon, O., *Solid State Ion*, **2020**, vol 344, 115138-115148
- 5 Badwal, S. *Solid State Ion* **1992**, 52 (1–3), 23–32.

Facet-dependent Carrier Dynamics of Cu₂O in Regulating the Photocatalytic H₂ Generation

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The emergence of well-defined architected photocatalysts has led to the realization of cuprous oxide (Cu₂O) as a promising photocatalyst due to its earth abundancy, ease in synthesis and band potential suitability for photoredox reactions.¹ In this regard, Cu₂O that can be activated by visible light is considered as a good candidate due to its appropriate conduction and valance band potentials. However, photocorrosion and rapid charge recombination are known to be the largest drawbacks of Cu₂O.² Our previous work systematically studied the photostability pathway of Cu₂O to mitigate the photocorrosion problems and have suggested that self-photooxidation of Cu₂O is the dominant photocorrosion pathway in a photocatalytic suspension system. Thus, the presence of hole scavenger was demonstrated to be vital in extracting holes from Cu₂O and suppressing its oxidation into CuO.³ Meanwhile, this study investigated the facet-dependent properties to further understand the charge transfer and separation within Cu₂O. With a stable Cu₂O photocatalyst, facet-dependent properties were revealed to play an important role in tuning the photocatalytic performance. Apart from the common facet-dependent properties (i.e. surface adsorption ability and surface electronic structures), the differences in surface defect density and charge carrier dynamics of each Cu₂O also alter the photocatalytic performance of Cu₂O. With proper morphological control of copper-based photocatalysts, photocatalytic performances can be enhanced. Apart from the understanding the photostability issues via systematic photocorrosion study, the effects of its facet-dependent properties towards photoreactivity were addressed.

References

1. Liang, X. Gao, L. Yang, S. and Sun, J. *Advanced Materials* **2009**, *21*, 2068-2071.
2. Toe, C. Y.; Scott, J.; Amal, R.; Ng, Y. H. *J. Photochem. Photobiol., C*, **2018**, *40*, 191-211.
3. Toe, C. Y.; Zheng, Z.; Wu, H.; Scott, J.; Amal, R.; Ng, Y. H. *Angew. Chem.* **2018**, *130*, 13801-13805.

Synergistic Cyanamide Functionalisation and Charge-Induced Activation of Nickel/Carbon Nitride for Enhanced Selective Photoreforming of Ethanol

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Photoreforming is a promising alternative to water splitting for H₂ generation due to the favourable organic oxidation half-reaction and the potential to simultaneously produce solar fuel and value-added chemicals.¹⁻³ Recently, carbon nitride has received significant attention as an inexpensive photocatalyst for the photoreforming process.^{4,5} However, the application of carbon nitride continues to be hampered by its poor photocatalytic performance. Herein, we report for the first time a synergistic modification of *in situ* photodeposited Ni cocatalyst on carbon nitride *via* cyanamide functionalisation and solid/liquid interfacial charge-induced activation by using excess Ni²⁺ ions. Synergism between the cyanamide functionalisation and charge-induced activation by the excess Ni²⁺ ions invokes enhanced activity, selectivity, and stability during ethanol photoreforming. A H₂ evolution rate of 2.32 mmol h⁻¹ g⁻¹ in conjunction with an acetaldehyde production rate of 2.54 mmol h⁻¹ g⁻¹ were attained for the Ni/NCN-CN. The H₂ evolution rate and elevated acetaldehyde selectivity (above 98%) remained consistent under prolonged light illumination. To understand the origin of the complementary promotional effects, the contributions of cyanamide groups and excess Ni²⁺ ions to selective ethanol photoreforming are decoupled and systematically investigated. The cyanamide functionality on carbon nitride was found to promote ethanol oxidation reaction *via* hole consumption, meanwhile enabling effective electron transfer to the Ni cocatalyst for H₂ evolution. Concomitantly, excess Ni²⁺ ions remaining in solution created a positively-charged environment on the photocatalyst surface which improved charge carrier utilisation and ethanol adsorption. The work highlights both the importance of carbon nitride functionality and charge on the photocatalyst surface in developing a selective photocatalytic reforming system.

References

1. Toe, C. Y.; Tsounis, C.; Zhang, J.; Masood, H.; Gunawan, D.; Scott, J.; Amal, R., Advancing Photoreforming of Organics: Highlights on Photocatalyst and System Designs for Selective Oxidation Reactions. *Energy Environ. Sci.* **2021**, *14* (3), 1140-1175.
2. Uekert, T.; Pichler, C. M.; Schubert, T.; Reisner, E., Solar-Driven Reforming of Solid Waste for a Sustainable Future. *Nat. Sustain.* **2020**, *4*, 383-391.
3. Ramis, G.; Bahadori, E.; Rossetti, I., Design of Efficient Photocatalytic Processes for the Production of Hydrogen from Biomass Derived Substrates. *Int. J. Hydrog. Energy* **2021**, *46* (22), 12105-12116.
4. Kasap, H.; Caputo, C. A.; Martindale, B. C.; Godin, R.; Lau, V. W.; Lotsch, B. V.; Durrant, J. R.; Reisner, E., Solar-Driven Reduction of Aqueous Protons Coupled to Selective Alcohol Oxidation with a Carbon Nitride-Molecular Ni Catalyst System. *J. Am. Chem. Soc.* **2016**, *138* (29), 9183-9192.
5. Uekert, T.; Kasap, H.; Reisner, E., Photoreforming of Nonrecyclable Plastic Waste over a Carbon Nitride/Nickel Phosphide Catalyst. *J. Am. Chem. Soc.* **2019**, *141* (38), 15201-15210.

Destabilization of magnesium hydride by embedding in TiH₂ matrix

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Magnesium is a promising hydrogen storage metal due to its high gravimetric and volumetric hydrogen uptake to form MgH₂ (7.7 wt%, 109 kg H₂/m³)¹. However, bulk Mg suffers from slow sorption kinetics and MgH₂ has a high thermodynamic stability with an equilibrium desorption pressure of 1 bar at 278°C². One strategy to overcome these hurdles is by Mg nanostructuring, as crystallite size reduction is expected to enhance hydrogen sorption kinetics and destabilize the hydride^{3,4}.

This work aims at embedding MgH₂ nanoclusters in a TiH₂ matrix. For that purpose, MgH₂- TiH₂ composites with Mg:Ti ratios between 20 and 60 mol% of Mg have been prepared by mechanochemistry under hydrogen pressure (P_{H₂} = 8 MPa)⁵. Their structural properties were determined by X-Ray Diffraction and hydrogenation properties measured in Sieverts' rigs. The crystallite size of MgH₂ phase decreases from 6 nm (Mg60%) to 2nm (Mg20%) with the increase of Ti-content, enhancing kinetics for reversible hydrogen sorption in Mg nanoclusters. Pressure-Composition-Isotherms of Ti-rich nanocomposites exhibit high hysteresis and thermodynamic destabilization as displayed in Figure 1. Complementary thermal characterisations by Temperature Programmed Desorption in closed systems and Thermal Desorption Spectroscopy under high vacuum (< 10⁻⁶ mbar) confirmed destabilization effects not only for MgH₂ nanoclusters but also for TiH₂ matrix.

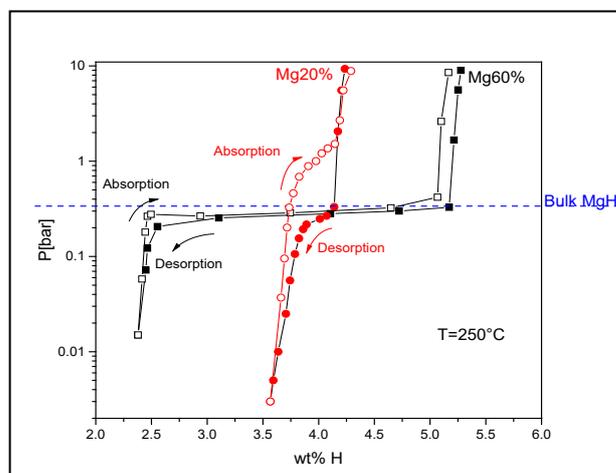


Figure 1: PCI absorption and desorption curves for Mg60% (60MgH₂-40TiH₂) and Mg20% (20MgH₂-80TiH₂) at 250°C

References

- ¹ V.-A. Yartys et al. *International Journal of Hydrogen Energy* 44. (2019) 7809.
- ² M. Hirscher, *Handbook of Hydrogen Storage*. John Wiley & Sons; 2010.
- ³ L. Pasquini, *Crystals* 8 (2018) 106.
- ⁴ N. Patelli et al. *Inorganics* 6.1 (2018): 13.
- ⁵ P. Rizo-Acosta, et al, *J. Mater. Chem. A*, 7 (2019) 23064 – 23075.

Investigation of structural evolution and hydrogen sorption properties of $Y_{0.9}Ni_{2-y}Mn_y$ ($0.1 \leq y \leq 0.5$) alloys with C15 Laves phase structure

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AB_2 -type alloys (A = Rare Earth or Early Transition Metal, B = Last Transition Metal) with the C15 Laves phase structure have more tetrahedral sites than AB_5 and AB_x ($3 \leq x \leq 3.8$) alloys. It allows to accommodate more hydrogen and provide high hydrogen storage capacity [1]. YNi_2 does not crystallize in the classic C15 Laves phase structure but in a vacancy-ordered superstructure with composition $Y_{0.95}Ni_2$. Upon hydrogenation YNi_2 suffers from hydrogen-induced amorphization or disproportionation [2] and becomes amorphous upon hydrogen absorption of 3 H/mol [3]. Thus, its reversible capacity and cycle life are low.

This work aims at stabilizing YNi_2 upon hydrogen cycling by substituting Mn for Ni in pseudo-binary $Y_{0.9}Ni_{2-y}Mn_y$ ($0.1 \leq y \leq 0.5$) compounds. Surprisingly, all these compounds crystallize in the classic C15 structure while maintaining Y sub-stoichiometry. As $Y_{0.95}Ni_2$ is stabilized by vacancy ordering of Y sites, one may expect that $Y_{0.9}Ni_{2-y}Mn_y$ compounds crystalize in the C15 phase with higher content of disordered Y-site vacancies.

Neutron diffraction measurements have been performed to determine atom occupancy in $Y_{0.9}Ni_{2-y}Mn_y$ compounds. Rietveld refinement of neutron data evidences no vacancies in the A -site and Mn occupation not only in the B site but, surprisingly, also in the A site. The fact that Mn can behave as an A -type atom has been previously observed in the $ZrMn_{2+x}$ and $TbNi_2Mn$ systems [4,5]. The hydrogenation properties of $Y_{0.9}Ni_{2-y}Mn_y$ compounds and their relationship with the crystal structure will be discussed.

References:

- [1] B. Kotur, O. Myakush, I. Zavaliy, Hydrogen Sorption Properties of Some $RM_{2-x}M_x$ and $RM_{2-x}Al_x$ ($R = Y, Gd, Tb, Er, Ho$; $M = Mn, Fe, Co, Ni$) Laves Phase Ternary Compounds, *Croat. Chem. Acta.* 82 (2009) 469-476.
- [2] U.-I. Chung, Y.-G. Kim, J.-Y. Lee, General features of hydrogen-induced amorphization in RM_2 ($R =$ rare earth, $M =$ transition element) Laves phases, *Philos. Mag. B.* 63 (1991) 1119–1130.
- [3] K. Aoki, T. Yamamoto, T. Masumoto, Hydrogen induced amorphization in RNi_2 laves phases, *Scr. Metall.* 21 (1987) 27–31. [https://doi.org/10.1016/0036-9748\(87\)90401-7](https://doi.org/10.1016/0036-9748(87)90401-7).
- [4] T. Kodama, H. Anada, H. Kaminaka, The site occupancies for the excess manganese atoms and the third element niobium in the intermetallic compound $ZrMn_2$, *J. Alloys Compd.* (1995) 6.
- [5] J.L. Wang, C. Marquina, M.R. Ibarra, G.H. Wu, Structure and magnetic properties of RNi_2Mn compounds ($R = Tb, Dy, Ho, and Er$), *Phys. Rev. B.* 73 (2006) 094436. <https://doi.org/10.1103/PhysRevB.73.094436>.

Electron migration mechanisms within covalently immobilised Co porphyrin-based catalysts for oxygen reduction reaction

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Electrocatalytic oxygen reduction reaction (ORR) is a multielectron, multiproton reaction taking place on the cathode of proton exchange membrane (PEM) fuel cells. Carbon-supported Co tetraphenylporphyrin (CoTPP) is an excellent ORR catalyst, however the reaction almost exclusively follows an undesirable $2e^-$ reduction pathway.¹ Hence, a method enabling $4e^-$ reduction mechanism on an otherwise efficient, but H_2O_2 -selective catalyst would be of high value for the renewable energy industry.

In this work we demonstrate that the selectivity of the porphyrin-based catalysts could be controlled via covalent immobilization of the complex on the electrode surface. Covalent grafting of the CoTPP was performed using potentiostatic electroreduction of the corresponding diazonium salt.²⁻³ The resulting **CoTPP-cov/10** electrode (where 10 is the electrografting time in min) demonstrates a selectivity to $4e^-$ reduction of 55 % in contrast to 0 % observed on noncovalent counterpart **CoTPP-noncov**. The H_2O_2 reduction also proceeds ~ 2.9 times faster on **CoTPP-cov/10**. The direct imaging of the surface redox kinetics using variable-frequency square wave voltammetry (VF-SWV) shows a strong outbound propagation of electrons across covalently grafted layer which results in ~ 9 times higher abundance of active sites compared to **CoTPP-noncov**. The improved charge transfer rate in turn increases the probability of multielectron reaction events (Figure 1a). Thus, the porphyrin-to-porphyrin bonds turn a simple molecular catalyst into an extended conductive macromolecular framework (Figure 1b). Such a structure provides a strong electron flux matching the inbound flow of O_2 and gives a longer residence time for the intermediates via a diffusion-mediated mechanism.

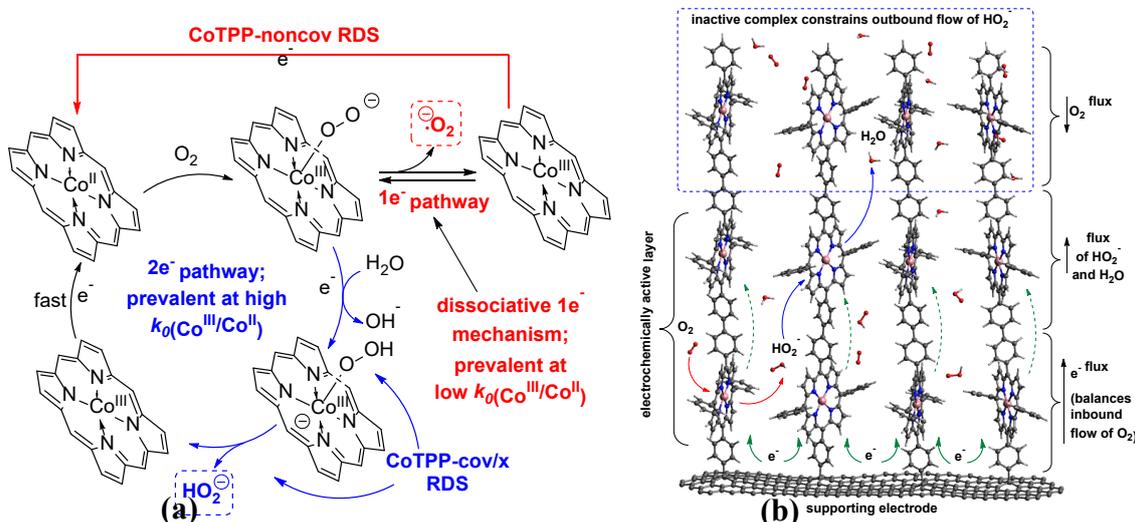


Figure 1: (a) Molecular and (b) macromolecular mechanisms of ORR on Co porphyrins.

References

- [1] Zhang, W.; Lai, W.; Cao, R., *Chem. Rev.* **2017**, 117 (4), 3717-3797
- [2] Marianov, A.; Jiang, Y., *ACS Sustainable Chem. Eng.* **2019**, 7, 3838-3848
- [3] Marianov, A. N.; Jiang, Y., *Appl. Catal. B* **2019**, 244, 881-888

Fabrication of bismuth-rich $\text{Bi}_3\text{O}_4\text{Br}_x\text{I}_{1-x}$ solid solutions for improved photocatalytic N_2 fixation in pure water

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Abstract:

As an alternative to the Haber-Bosch process, photocatalytic N_2 reduction under ambient condition is a reassuring strategy for energy conversion and storage. This work developed a novel bismuth-rich $\text{Bi}_3\text{O}_4\text{Br}_x\text{I}_{1-x}$ solid solution photocatalyst for N_2 fixation under ambient conditions. The results show that $\text{Bi}_3\text{O}_4\text{Br}_{0.5}\text{I}_{0.5}$ exhibits the best activity, 6.308 mmol/L.g, without using any sacrificial agent. The presence of oxygen vacancies in the fabricated samples was evidenced by XPS spectra. The bandgap of the photocatalysts became narrower by changing the ratio of Br/I from 1 to 0.25 in $\text{Bi}_3\text{O}_4\text{Br}_x\text{I}_{1-x}$ samples, and the morphology was shifting nanosheets to nanorods structure. BET and TPD- N_2 analysis show that $\text{Bi}_3\text{O}_4\text{Br}_{0.5}\text{I}_{0.5}$ provides not only the higher surface area available for the photocatalytic reaction and but also offers the higher N_2 adsorption and active sites. $\text{Bi}_3\text{O}_4\text{Br}_{0.5}\text{I}_{0.5}$ shows better separation of photogenerated electron-hole pairs compared to other samples based on photoelectrochemical analysis. Furthermore, $\text{Bi}_3\text{O}_4\text{Br}_{0.5}\text{I}_{0.5}$ shows an excellent structural stability in photocatalytic N_2 fixation. A reaction pathway of the photocatalytic N_2 fixation process was proposed for based on the above analysis. This research opens a new way to develop high-performance photocatalysts for ammonia generation.

END OF BOOK