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ABSTRACT BOOKLET



Australian Research Council
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Green Electrochemical Transformation
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Aaron Marshall

Fancy electrocatalysts vs well-designed electrocatalytic systems

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Electrocatalytic reduction of CO₂ has the potential to convert CO₂ into carbon-based fuels by using renewable energy. While a wide range of electrocatalytic materials have been investigated, the process is still limited by poor reaction selectivity, large overpotentials and low reaction rates. Therefore there are now many research groups studying a huge range of electrocatalytic materials (metals, oxides, carbon nitrides, molecular complexes) to improve the performance of this important process. Over the last 10 years, our laboratory has investigated many electrocatalysts based on Cu, Co and Au, and while selectivity and activity are clearly influenced by the nature of the electrocatalyst, large differences in the CO₂ reduction behaviour can be achieved by simply altering the mass transfer (electrolyte and CO₂ flow, electrode porosity and geometry, and local gas evolution) at the electrode-electrolyte interface. These changes in mass transfer effect both reactant and product transport and the local pH at the electrode surface, and not only affect the current density (when switching from conventional aqueous H-cells to gas-diffusion electrode cells, the enhanced mass transport can increase the current densities by two-orders of magnitude) but also product selectivity. This suggests there are some limitations in what can be learnt from aqueous based electrocatalytic testing and that there are complex interconnected factors which govern CO₂ reduction behaviour. Ultimately understanding these factors is critical in developing better electrocatalytic systems and not just fancy electrocatalysts.

Biography



Aaron Marshall is a Professor in Chemical and Process Engineering at the University of Canterbury, New Zealand. He received bachelor and master degrees from Massey University in New Zealand and a PhD from the Norwegian University of Science and Technology. Aaron specialises in electrochemical engineering and currently works on CO₂ reduction, water electrolysis, flow batteries and molten oxide electrolysis. Professor Marshall has co-founded two companies related to his research and is passionate about converting science into practical applications which can make a difference.

Adam Lee

Multimetallic catalysts for CO₂ methanation

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Green hydrogen from water electrolysis affords an economic route to renewable chemicals and fuels via thermocatalytic CO₂ hydrogenation (power-to-gas-concept).¹ CO₂ methanation may employ precious or non-precious transition metals, with the former being more active and selective.² However, precious metal thrifiting and improved stability are required to lower costs. Here we discuss a bimetallic Ni@Rh core-shell catalyst prepared by galvanic replacement (GR) which enhances CO₂ methanation versus an analogue prepared by chemical reduction (CR) or monometallic Rh/Al₂O₃ (**Figure 1**)³ Superior performance of RhNi/Al₂O₃ (GR) is attributed to Rh dispersion as an atomically thin RhO_x shell, stabilised by a strong Rh-Ni interaction. Operando IR spectroscopy identifies reactively-formed CO from the dissociative chemisorption of CO₂ over Rh as the key intermediate for methane production. Surface formate, from the dissociative chemisorption of CO₂ and subsequent hydrogenation over alumina, is a catalytic spectator. This mechanistic insight paves the way to high activity nanostructured catalysts for CO₂ methanation.

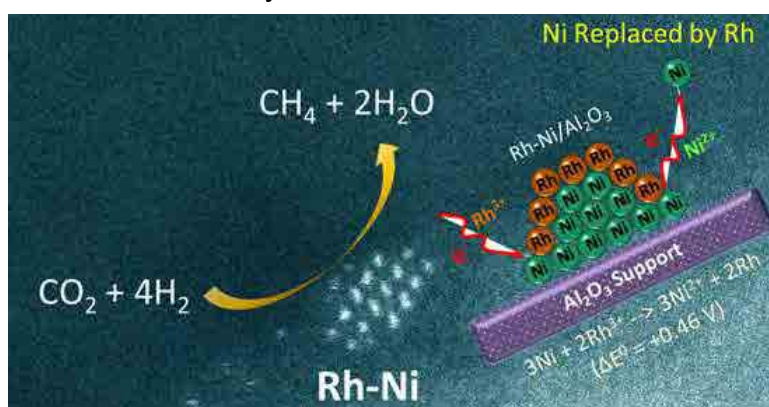


Figure 1. Bimetallic Ni@Rh core-shell catalyst for CO₂ methanation.

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Biography



Adam is Professor of Sustainable Chemistry at Griffith University, and has previously held Chair appointments at RMIT, Aston, Warwick, Monash and Cardiff Universities. He has published >300 peer-reviewed articles, received the 2023 RACI Welcome Award and the 2012 Beilby Medal and Prize of the Royal Society of Chemistry for his contributions to catalysis, green chemistry and materials science, and is Editor-in-Chief of *Materials Today Chemistry*.

Adrian Sheppard

Directions in 3D and 4D Imaging for Characterising Materials and Processes

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Tomographic imaging methods, using x-rays, electrons, neutrons or even visible light, can non-destructively provide detailed 3D maps of internal structure on a range of length scales, even down to the nanoscale. *In-situ* tomography – for example to capture gas bubble formation in the porous transport layer in electrolysers – has great potential for helping understand and improve electrolyser performance. However, these methods, while powerful, have challenges and limitations and have not yet fulfilled their potential in many areas.

In this talk we provide an overview of 3D and 4D microscopy techniques that are most relevant to electrolysers and carbon utilisation applications, and highlight some recent advances in the technology along with potential future directions. We focus particularly on *in-situ* techniques and 4D tomography for mapping dynamic processes.

We also discuss the challenges of analysing enormous 3D/4D data sets and provide examples where deep learning is proving transformational, through algorithms that can be less subjective, more accurate and less labour intensive than was previously possible. These tools are progressively becoming more accessible to a wider range of users.

Biography



Adrian Sheppard is professor and X-ray Imaging group leader in the Department of Materials Physics in the Research School of Physics at ANU. He completed his PhD in Physics at the Australian National University (ANU) in 1996 has held research positions at the Université Libre de Bruxelles, the University of New South Wales and the Australian National University. His research interests include tomographic and computational imaging, parallel algorithms for image processing, understanding complex morphology, and fluid flow through porous media in biology, geology and materials science.

Ahmad Md Azmi

Bimetallic Synergies of Ni and Fe on Al₂O₃ Catalysts in a Hybrid Thermal-Plasma Catalytic System for CO₂ Methanation

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The intensification of natural disasters has raised worldwide concerns over climate change with anthropogenic CO₂ being the main cause. Research surrounding CO₂ mitigation through carbon capture, storage and utilization is being increasingly explored to mitigate anthropogenic climate change. One approach to CO₂ utilization, to reduce CO₂ emissions while generating added value products, is CO₂ methanation (CO₂ and H₂ to CH₄). However, thermodynamic limitations constrain the scalability of this process for industrial applications. Hence, non-thermal plasma (NTP) has become a topic of interest in catalytic research as the non-equilibrium nature of the plasma produces high energy species while maintaining low bulk temperatures. Although plasma methanation has demonstrated successful conversions of CO₂ into CH₄, a noticeable gap is still prevalent in research around catalytic properties driving the reaction. As such, the mechanism of plasma methanation remains obscure. This work examines bimetallic Ni and Fe supported by Al₂O₃ under thermal and plasma methanation conditions to elucidate catalyst characteristics critical for plasma methanation. To understand the role of the metals, bimetallic catalysts with Ni and differing amounts of Fe were produced via wet impregnation (WI) and deposition precipitation (DP) to vary metal-metal interactions. For both synthesis methods, catalysts with small amounts of Fe demonstrated peak performances, in terms of CO₂ conversion and CH₄ selectivity, under thermal conditions. Conversely, under plasma conditions, by varying metal-metal interactions, the plasma performance was tuned. WI catalysts performed the best with higher amounts of Fe, whereas DP catalysts peaked with small to moderate amounts of Fe. This was attributed to the change in the electronic properties of the catalysts, observed to be more critical for plasma methanation. This study provides a substantial move towards a greater understanding of catalyst design for plasma enhanced CO₂ methanation, resembling a step forward to making methanation a more sustainable means of CO₂ utilization.

Biography



Ahmad Zhafran Bin Md Azmi is a dedicated 2nd-year Ph.D. student affiliated with the prestigious PartCat Research Group at the University of New South Wales (UNSW). His current research focuses on CO₂ utilization, with a particular emphasis on processes related to CO₂ reduction. As an emerging researcher in the field, Ahmad is passionately committed to addressing the critical challenge of creating a more sustainable future for all. In addition to his research pursuits, he aspires to become a future educator, with the aim of sharing his knowledge and inspiring the next generation of researchers. Ahmad is enthusiastic about his journey in the research arena and is eager to absorb knowledge and experiences along the way.

Aijun Du

Computational Design of new Catalysts for the Reduction of Carbon Oxide into Multi-carbon Product

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Materials catalytic properties are in principle determined by electronic functionalities. Now quantum mechanics-based ab initio simulations allow us the accurate calculation of those functionalities, shining light “from the bottom up” – on the structural, thermodynamic, and kinetic aspects of catalytic processes – facilitates the selection and rational design of efficient catalysts among candidate materials. In this presentation, we will choose some examples from my recent research showing how electronic functionality modulations via controlling symmetry [1], interface [2], ligand functionalization and catalyst-catalyst separation [3] can help the development of carbon oxide reduction catalysts for producing high valued multi-carbon fuels.

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Biography:



Aijun Du received PhD in 2002 from Fudan University of China and is currently a full professor at Queensland University of Technology. He was awarded both ARC Future and QEII fellowships. His research lies at the interface of chemistry, physics, and engineering, focusing on the development of innovative materials for energy, environmental and nanoelectronics applications using advanced theoretical modelling. He has published 400 refereed journal papers. His works have been cited 31,000 times with an H-index of 86. He has been a Clarivate highly cited researcher since 2020.

Akshat Tanksale

Aqueous Phase Conversion of Carbon Dioxide into Acetic Acid

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Global production of acetic acid exceeds 6.5 million tonnes per annum, however, currently it is predominantly synthesized via carbonylation of methanol, in which both carbon monoxide and methanol are fossil-derived (typically from natural gas). Sustainable production of acetic acid (AA) via carbon dioxide hydrogenation to make methanol, followed by hydrocarbonylation of methanol with CO₂ and H₂ is a highly attractive alternative. Another alternative is direct hydrogenation of CO₂ into formic acid and subsequently acetic acid. CO₂ transformation into AA is highly desirable to achieve net zero carbon emissions, but significant challenges remain to achieve this efficiently. In this presentation we report a range of heterogeneous catalysts, thermally transformed metal organic frameworks, based on iron, cobalt and nickel metal centres, for highly selective AA formation via methanol hydrocarboxylation or direct hydrogenation. We recently reported a maximum yield of AA to be 590.1 mmol/g_{cat}.L with 81.7% selectivity at 150 °C in the aqueous phase using Lil as a co-catalyst [1]. Both the reactions are believed to proceed via formic acid intermediate. This work is scalable and industrially relevant for CO₂ utilisation to reduce carbon emissions, especially if green methanol and green hydrogen are used.

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Biography



Prof. Akshat Tanksale is a Professor at the Department Chemical and Biological Engineering at Monash University and concurrently holds the positions of Carbon Theme Leader at the Woodside Monash Energy Partnership, and Deputy Director of the ARC Research Hub for Carbon Utilisation and Recycling. He leads the Catalysis for Green Chemicals group at Monash University, pioneering CO₂ conversion into C₁ bulk chemicals such as syngas, formaldehyde and its derivatives, and acetic acid. Working alongside Woodside, and other industries on research on CO₂-to-products, he is the lead inventor on 3 patents on CO₂ conversion, in addition to 4 other patents on circular economy. He has published over 65 papers in high impact journals and serves as an Associate Editor of Frontiers of Chemical Engineering and Sustainability journals. He is a recipient of the Caltex Award of Excellence in Chemical Engineering 2018.

Alexis Bell

Electrochemical Reduction of CO₂: Challenges for Materials and System Design

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The electrochemical reduction of CO₂ holds considerable potential as a means for converting CO₂ emitted from stationary sources and ultimately from the atmosphere into fuels and chemicals using renewable energy sources (e.g., wind, solar radiation). The challenge is to select the required materials and to design electrochemical reactors that can accomplish this goal economically. While considerable insight into the effects of catalysts and electrolyte selection have been achieved in laboratory studies using H-cells or flowthrough compression cells, such devices cannot achieve the current densities needed for industrial scale (> 100 mA/cm²). This talk will first review what has been learned from laboratory studies concerning the effects of catalyst composition and structure as well as electrolyte composition on the activity and selectivity of Cu and Ag catalysts for CO₂ reduction and the factors affecting product current density. It will then be shown that to meet the demands of industrial-scale operation, it is necessary to consider membrane electrode assemblies (MEAs). The structure of the MEA involves an ionomeric polymer membrane as the electrolyte, coated with an anode catalyst layer (aCL) on one side and a cathode catalyst layer (cCL) on the other side. A hydrated stream of CO₂ is supplied to the cCL through a gas diffusion layer and an aqueous stream of electrolyte is supplied on the backside of the aCL. Experimental work has shown that the ionomer membrane and the ionomer in which the catalysts are imbedded must be fully hydrated to maintain high ionic conductivity through these elements to lower the voltage required for a given current density. This presentation will end with an illustration of the challenges that must be met to design an MEA.

Biography



Dr. Bell is currently Professor Emeritus in the Department of Chemical and Biomolecular Engineering at the University of California, Berkeley and is an Affiliate at the Lawrence Berkeley National Laboratory. He received his B.S. and Ph.D. degrees in chemical engineering from the Massachusetts Institute of Technology. His research specialty is catalysis and chemical reaction engineering with an emphasis on understanding the fundamental relationships between catalyst structure and composition and catalyst activity and selectivity. The objectives of his program are pursued through a combination of experimental and theoretical methods, enabling the attainment of a deeper understanding of the core issues of interest than can be achieved by using either approach alone. Dr. Bell has published nearly 800 papers for which he has received numerous national and international recognition. Dr. Bell is a member of the **National Academy of Sciences**, the **National Academy of Engineering**, a Fellow of the

American Association for the Advancement of Science, a member of the **American Academy of Arts and Sciences**, and a foreign member of the **Russian Academy of Sciences**.

Alfred Bekoe Appiagyei

Fly ash waste-derived ferrite for Superior chemical looping dry methane reforming

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The chemical looping methane dry reforming has been re-emerging as a cost-effective technology with significant promise and potential for carbon neutrality. However, the lack of eager pursuit for high-performance but stable oxygen carriers stifles its progress. Fe₂O₃-based oxygen carriers have been examined thoroughly but suffer low oxygen transfer capabilities and sintering-induced deactivation at high temperatures during cycling. In this work, we illustrate the development of synergistic promotions of Mg, Al, Ca, and traces of Mn and Ti on the oxygen transfer rate of Fe₂O₃ in an oxide complex synthesised from an otherwise global waste, fly ash from pulverised coal. With systematic characterisations including high-temperature X-ray diffraction (HT-XRD) and medium energy X-ray absorption spectroscopy (MEX-1) beamlines from Australia synchrotron, we reveal that the reduction of CH₄ and oxidation of CO₂ is enhanced by the participation of unique spinel solid solution that hinders any irreversible structural transformation during redox cycles. Specifically, the oxygen carrier records a superior oxygen uptake-to-release ratio of 0.97 and excellent stability over ten repeated cycles exceeding that of commercial Fe₂O₃. The high oxygen transfer rate controlled by the synergy of multiple oxides coupled with the high textural material plays an essential role in the high syngas selectivity. This approach of oxygen carrier design offers a fresh path to utilize waste and tailor the oxygen activities of carriers for chemical looping.

Biography



Alfred Bekoe Appiagyei is a Ph.D. student in the Department of Chemical and Biological Engineering, at Monash University. Prior to the PhD program, Alfred received an MSc degree in Energy Engineering from Dongguk University, South Korea where he researched on supercapacitors. Currently, he is focusing on developing Fe-based catalysts from Victorian fly ash waste as oxygen carriers to convert CO₂ and CH₄ into syngas through the chemical looping dry methane reforming.

Aloka Kumar Sahu

Photo- and Electrocatalytic CO₂ Reduction based on Ga-doped NiTiO₃ Perovskite Nanoparticles

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Efforts to develop efficient catalysts capable of accelerating the light-driven electrochemical CO₂ reduction reaction (CO₂RR) hold significant promise for advancing sustainable technologies by storing solar energy in the form of energy-dense carbon fuels.^{1,2} The coexistence of activity and durability within a photoelectrocatalyst presents a challenge, often leading to a trade-off between these properties. To address this, strategies of hybrid heterostructures, composition modulation, and defect engineering have been widely investigated.³ Titanate perovskites exhibit commendable photocatalytic activity and robustness⁴, yet they falter as effective electrocatalysts, thus impeding their practical utility. In this work, we applied another direction of material design, which adopted a semiconductor-based perovskite NiTiO₃ (NTO) photoelectrocatalyst, which is highly stable in an alkaline medium. Through doping of Ga to extent ~1 wt. % (relative to Ti) into NTO and loading of a small quantity of noble metal cocatalyst, this composite photoelectrocatalyst can exhibit better CO₂RR performance and durability than NTO. With the information from the characterisation of the electronic structures and the photoelectrochemical measurement of Ga-doped NTO (GNTO) as direct evidence, lattice oxygen vacancy sites synergistic with small resistivity increased the CO₂RR activity. Additionally, the photoelectrocatalytic performance of GNTO can be further optimized by Ru metal loading, which improves the separation of photoinduced electrons and holes and provides more active sites for CO₂RRs. This study presents a perovskite-based photoelectrocatalyst for the reduction of CO₂ and provides valuable insights into the reconstruction of optoelectronic properties of semiconductors in catalytic reactions for energy-related technologies.

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Biography

Aloka Kumar Sahu is currently pursuing a PhD in a joint program between the School of Chemical Engineering, The University of Queensland, Australia, and the Department of Chemical Engineering, Indian Institute of Technology Delhi, India. He is jointly supervised by Prof. Sreedevi Upadhyayula and A/Prof. Thomas E Rufford. He also obtained his Integrated B.Tech and M.Tech Dual Degree in Chemical Engineering from National Institute of Technology Rourkela, India. His research focuses on developing visible-light-driven photocatalysts and photoelectrodes for carbon dioxide reduction.

Anoja Kawsihan

Production of C₂+ products through the Electrochemical Reduction of CO₂ by Single atom Fe decorated Cu nano-dendrites

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The pursuit of producing C₂+ products while simultaneously capturing atmospheric CO₂ has emerged as a compelling goal within the contemporary research. Existing catalysts for CO₂ reduction can achieve high selectivity toward CO, yet they often lack a high efficiency for generating C₂+ products. Copper based materials have attained substantial interest because of the capability to convert CO₂ to multiple products, coupled with the adjustable selectivity achievable by manipulating Cu structures. Among the Cu based catalysts, Cu dendritic nanostructures are providing more active sites to promote the conversion of CO intermediate to C₂+ products because of the rich local stress & strain effects and exposed undercoordinated surface sites. When combined with other catalysts or materials, such as carbon-supported iron single-atom catalysts, dendritic copper structures can experience synergistic effects that further enhance their catalytic activity and selectivity for CO₂ reduction. Herein, we prepare the copper dendrite nanostructures decorated by carbon supported iron single atom catalysts, aiming at promoting CO₂ reduction toward multiple products. Scanning electron microscope (SEM) exhibits the dendrite nanostructure morphology of Cu substituted on carbon paper. The porous structure of the prepared iron single atom on carbon substrate derived from Fe-doped zeolitic imidazole framework-8 (ZIF-8) determined by the SEM image. The Fe³⁺ ions are expected to coordinate to pyrrolic nitrogen atoms and will promote the conversion of CO₂ to CO, followed by the further reduction to C₂+ products on Cu dendrite nanostructure. The electrochemical behaviour under CO₂ reduction conditions is elucidated by linear sweep voltammetry (LSV) and amperometry test results. Subsequent performance testing and mechanistic investigations are anticipated in the upcoming stages. This project will address the current issue in expanding CO₂ reduction to industrial level with compromising limitations of existing electrocatalyst.

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Biography



Anoja Kawsihan is now High degree Research student under the supervision of Prof. Zaiping Guo and the Co-supervision of Jinshuo Zou at The University of Adelaide, SA 5005 Australia. I am MPhil Graduate in Nano and Advanced Technology. I have completed my MPhil degree in 2021 at Sri Lanka Institute of Nanotechnology, Homagama, Sri Lanka. I received Bachelor degree in Mineral Resources and Technology and specialized in Mineral Processing Technology in 2017 at Uva Wellassa University, Badulla, Sri Lanka. My previous research projects mainly focus on value addition of minerals using advanced technology such as Mica, Garnet, Feldspar, Apatite, Titanium and Graphite. My research publications include 2 published papers in high indexed international and national journals, 1 book chapter and 11 conference papers. I am a growing young researcher.

Aoni Xu

Theories for Electrolyte effects in CO₂ electro-reduction

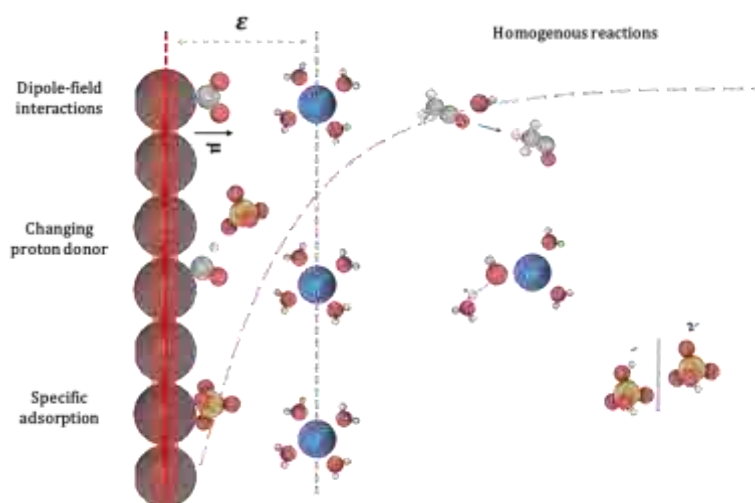
Aoni Xu

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The electrolyte can have a significant impact on eCO₂R activity and selectivity and its optimization is a critical part of electrolyzer design. I will discuss recent work on electrolyte effects in eCO₂R including the effects of the cation, anion and the electrolyte pH, both from the experimental and theoretical front, and provide our viewpoint of future directions for investigations on this topic and possible strategies for improving eCO₂R performance via electrolyte optimization.

As summarized in the conspectus graphic, the electrolyte influences eCO₂R activity via, (1) **dipole-field interactions**: metal cations establish an interfacial electric field, which stabilizes intermediates with large dipole moments; at a higher pH a given RHE potential corresponds to a more negative absolute field, thereby a stronger stabilizing field, (2) **homogeneous reactions**: cations can undergo hydrolysis reactions which tune the interfacial pH; buffering anions react with OH⁻ produced from eCO₂R which regulates pH; the formation of CH₃COO⁻ arises from the reaction of OH⁻ with a ketene intermediate in solution phase, (3) **shifts in proton donor**: hydronium, anions, and water can all act as proton donors, and the predominant proton donor depends on the intrinsic kinetics and mass transport, and (4) **surface poisoning**: phosphate anions poison Cu surface by specific adsorption at low overpotentials



So far, the existing models of electrolyte effects rationalize various experimentally observed trends, having yet to demonstrate general predictive capabilities. The major challenges of i) the long time-scale associated with a dynamic, ab initio picture of the catalyst | electrolyte interface, and ii) the overall activity determined by the length-scale interplay of intrinsic microkinetics, homogeneous reactions and mass transport limitations, require both computational methodologies development and ample communications between experiments and simulations.

Biography

Aoni Xu is a postdoctoral fellow at CatTheory center, under supervision from Prof Jens Nørskov. Before joining CatTheory, she is an alumna of Sargent group. Her research interest is focused on atomistic and continuum level modeling of electrochemical interfaces with applications in sustainable energy conversion.

Benjamin Muir

Introducing CSIROs robotic and automated capabilities that enable rapid, materials synthesis, formulation, screening and optimisation

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Could you utilise CSIROs resources in your catalyst research? This presentation will aim to inform you of the skill sets CSIRO staff have and the laboratory equipment and facilities we maintain that may enable you to produce and potentially screen a whole lot more catalysts than you may have thought possible. The presentation will use a few science examples to highlight our research capabilities and highlight the fact that use of, Automation, Artificial Intelligence and Machine Learning algorithms are now playing a large role in assisting our research projects.

Biography



Dr Muir and Dr Fong are Senior Research Scientists in CSIRO Manufacturing with over 40 years of combined experience conducting materials science research including the generation of and screening of catalyst libraries. Dr Muir has over 10 patents and 100 journal publications and has successfully commercialised a number of technologies across a broad range of research domains from aerospace to health. He and Celesta run the Rapid Automated Materials & Processing Centre at the CSIRO laboratories in Clayton, Melbourne. We look forward to collaborating with scientists in the CoE on catalyst synthesis.

Bernt Johannessen

Advanced Materials meets X-ray Absorption Spectroscopy: a Strong and Growing Partnership

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X-ray absorption spectroscopy (XAS) is a versatile technique for probing the local atomic structure and oxidation states in various sample types, including solids, liquids, nanoscale, or single-atom materials. The XAS Beamline at the Australian Synchrotron in Melbourne has experienced a growing demand for access from the *Advanced Materials* community, broadly speaking *catalysis* and *energy storage*. This demand has been amplified by the ability to do *in situ* measurements [1, 2]. Due to the strong demand and limited beamline access, we have recently implemented measures to enable more researchers to access our facility, increase scientific output, and enhance societal benefits. These measures include, for example, energy slew scanning, efficient operations, and the introduction of new beamlines coming online. In my presentation, I will demonstrate the changes we have witnessed in our user community over the past decade, showcase the capabilities of the XAS Beamline, and provide a future direction.

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Biography



Bernt Johannessen completed his undergraduate studies at the University of Auckland, New Zealand, and later earned a PhD from the Australian National University in Canberra. He has been involved with X-ray Absorption Spectroscopy and related techniques for over 20 years, including the over 15 years as a beamline scientist. He now holds the position of Senior Scientist and Beamline Responsible at the XAS Beamline in Melbourne. His academic interests include Catalysis and Energy Storage.

Brian Seger

An overall analysis of CO₂ and CO electrolysis devices

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This talk will analyze CO₂ electrolysis from a device perspective to provide perspective into what are the bottlenecks in the field and how to resolve them. While we show CO₂ can effectively be converted into CO, ethanol and ethylene, this electrochemical reduction process produces hydroxyl groups, which can additionally convert CO₂ to carbonates. Via a device mass balance, we show these carbonates transfer through a membrane, get acidified at the anode, and are released as CO₂ along with O₂.¹ The CO₂ released anodically is more than the CO₂ converted to products at the anode entailing this is a substantial issue.

An additional issue is that during higher current density (>100 mA/cm²) CO₂ electrolysis devices are prone to cathodic 'flooding' leading to greatly enhanced hydrogen production. We show that during this degradatory issue there is chaotic oscillatory fluctuations in potential, and product distribution.² By analyzing these fluctuations in the presence of a synchrotron, we monitor salt deposition and even electrolyte penetration by a shift in the background scattering signal. From the comprehensive analysis we have developed a hypothesis of why we both see the oscillations as well as flooding. Interestingly, salt solubility and precipitation has a strong role in flooding issues. We then analyzed various salts (Li, Na, K, Cs) of differing solubility while doing CO₂ electrolysis.³

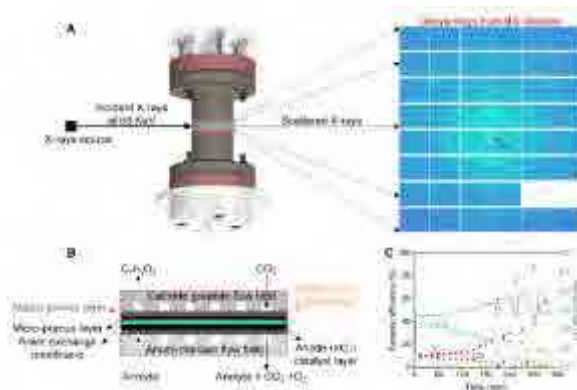


Figure 1: Synchrotron cell and the oscillatory degradation we analyze with it. From Ref 2.

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Biography



Brian Seger received his B.Sc in Chemical Engineering from the University of Toledo in 2003, and worked with Prashant Kamat at the University of Notre Dame where he received his PhD in 2009. After a year post-doc with Lian Zhou Wang in the University of Queensland, he started at DTU Physics as a postdoc and is now a full professor in Physics. His earlier work focused on fuel cells and photoelectrochemistry, with more recent work focusing on electrosynthesis studies particularly related to CO₂ and CO electrolysis.

Calvin Yuen Leong Chow

Realising Catholyte-Free CO₂ Electrolysis Under Acidic Condition

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Electrochemical reduction of CO₂ (CO₂ER) is one of the promising approaches in realising sustainable, efficient CO₂ conversion into value-added products such as CO thereby closing the anthropogenic-driven carbon cycle. Despite the development of anion membranes for CO₂ER, their commercial application is hindered by CO₂ crossover due to carbonate formation. Therefore, operating CO₂ER in acidic electrolyte environment is gaining traction despite the prevalence of H₂ evolution reaction (HER). While the presence of alkali cations in an aqueous medium enables CO₂ER catalytic activity by coordinating reaction intermediates, it limits the cell operating temperature and induces salt precipitation that reduces cell reliability especially during continuous operations. Studies have shown that manipulating flow cell design, developing functional ligands for single atom catalysts (SACs) and ionomer composition are effective in suppressing HER, improved selectivity for protonation as well as reducing the reliance on cations for CO₂ electrolysis in acidic media. By pushing the operating temperature beyond the boiling point of water solvent of 100 °C, the added energy is postulated to enable better conversion coupled with improved stabilization intermediates brought by catholyte-free development. This poster hopes to demonstrate our current focus in examining CO₂ conversion activities under elevated conditions.

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Biography



Yuen Leong Chow recently completed his 1st year studies in PhD Engineering from the Department of Chemical and Biological Engineering. His research targets the development of scalable yet sustainable CO₂ER technologies, with the aim of realising acidic based electrolyte operations that promote better protonation of CO₂. Furthermore, he engages in mentorship programmes designed to nurture passion for STEM subjects amongst graduate students. In his free time, he enjoys reading; in particular journals, history, and sci-fi. Hailing from Malaysia, he sticks to his roots - having an immense love for food, by exploring different culinary fares.

Cameron Bentley

Nanoscale Structure–Activity Mapping of Electrocatalysts

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All solid surfaces—from the simplest monocrystals to the most complex composite nanomaterials—possess some degree of heterogeneity but determining how surface structure affects electrode functional properties (e.g., catalytic activity, selectivity, stability *etc.*) can often be challenging using traditional “bulk” electrochemical techniques. Scanning electrochemical cell microscopy (SECCM) is a nanopipette-based scanning probe microscopy (SPM) technique that utilises a mobile droplet cell to measure and visualise electrochemical (electrocatalytic) activity with high spatiotemporal resolution. This presentation will spotlight the use of SECCM for probing the electrocatalytic activity of nanomaterials on a commensurate scale to surface structural heterogeneities (*i.e.*, nm– μm scale). It will be demonstrated that this approach is widely applicable to: well-defined monocrystals (e.g., transition metal dichalcogenides: MoS₂ and WS₂); structurally and/or compositionally heterogeneous polycrystals (e.g., polycrystalline Pt, Pd, Cu, *etc.*) and; composite nanoparticle-on-support “ensemble” electrodes [e.g., $\beta\text{-Co(OH)}_2$ nanoplatelets supported on carbon]. In particular, it will be emphasised how nanoscale-resolved information from SECCM is readily related to electrocatalyst structure and properties, collected at a commensurate scale with complementary, co-located microscopy/spectroscopy techniques (e.g., SEM, TEM, EBSD, AFM *etc.*), to allow structure–activity relationships to be assigned *directly* and *unambiguously*.

Biography



Dr Cameron L. Bentley obtained his PhD from Monash University, Australia (2012 – 2015) and worked as a (Senior) Research Fellow at the University of Warwick, UK (2016 – 2020), supported by subsequent Endeavour (Australia), Marie Skłodowska-Curie (EU) and Ramsay Memorial (UK) Fellowships. Currently, he is an ARC DECRA Fellow at Monash University and his research centres on combining cutting-edge electrochemical imaging techniques with co-located microscopy/spectroscopy to solve contemporary structure–function problems in electromaterials science. Cameron has published >60 peer-reviewed articles and is the recent recipient of the *2020 Early Career Analytical Electrochemistry Prize of ISE Division 1* (International Society of Electrochemistry, ISE) and *2023 AM Bond Medal* (Electrochemistry Division of the Royal Australian Chemical Institute, EDRAI). He is also a Member of the Early Career Advisory Board of the peer-reviewed journal, ChemElectroChem (Wiley) and is a VIC State Representative on the committee of EDRAI.

Chen Jia

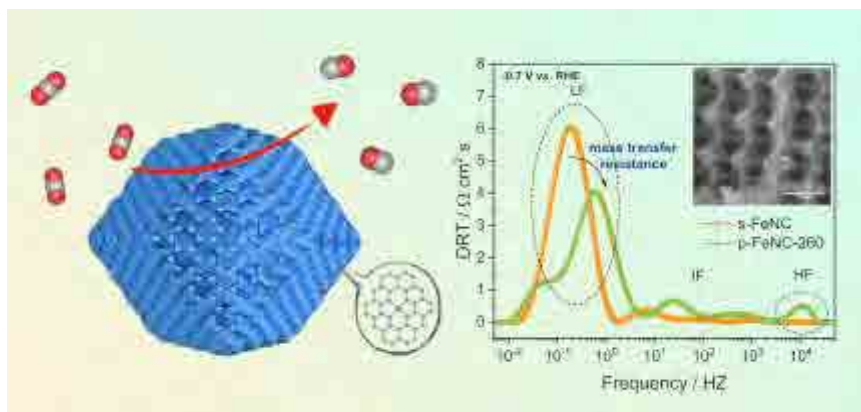
Ordered Hierarchical Porous Single-Atom Catalyst with Enhanced Mass Transfer for CO₂ Electroreduction

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Electrocatalysts are crucial to lower the energy barrier, tune the intricate reaction pathways and suppress competitive side-reaction.[1] Metal-nitrogen co-doped carbon single-atom catalysts (SACs), are one of the most promising candidates for CO₂RR due to their high intrinsic activity, maximum exposed active sites, and excellent stability.[2] Beyond the efficient active sites and advantageous local environment, a rapid mass transfer ability is also necessary during the catalyst design. The CO₂RR involves gas phase CO₂, liquid phase electrolyte and solid phase catalyst surface. The mass transport properties of catalysts such as the diffusion of reactant and products not only influence the rate of the reaction but also have significant impacts on the final activity and selectivity.[3] This is particularly important for SACs because of the limited active sites. However, there is little research that investigates in detail the mass transfer process in CO₂RR, and exposes the real relationship between mass transfer and final performance of SACs. In this work, we design a single-atom Fe-N-C catalyst with a highly ordered hierarchical porous morphology containing micropores, mesopores and macropores to maximum facilitate mass transfer process. By appropriate experimental design, *operando* electrochemical impedance spectroscopy and advanced distributed relaxation times analysis and pore-scale numerical simulations, we expose the morphology - mass transfer - performance interrelationship.



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Biography



Dr Chen Jia received his PhD degree in Chemistry in 2021 from the University of New South Wales Sydney supervised by Prof Chuan Zhao. He is currently working as a postdoctoral fellow in the same group. His research interests include the development of novel metal nanomaterials and single-atom catalysts, as well as their applications in the energy storage and conversion.

Chuan Zhao

Single-atom catalysts for electroreduction of CO₂

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The electroreduction of CO₂ (CO₂RR) is a sustainable approach to mitigate the raised global CO₂ emissions and further produce valuable chemicals. Electrocatalysts are crucial to lower the energy barrier, tune the intricate reaction pathways and suppress competitive side-reaction. In this presentation, I give a brief overview of our journey in the design of efficient catalysts for CO₂RR, from bulk metal to nanoparticles to single-atom catalysts (SACs). I summarize our progress in the design of efficient single-atom catalysts with advanced metal sites, novel coordination environments, porous substrates and synthesis routes. I will highlight the importance of reaction environment and provide an ionic liquids nanoconfinement strategy for local environment modification. In the end, I will provide some views and perspectives on the challenges and opportunities for using single-atom catalysts for CO₂RR towards industry.

Biography



Chuan Zhao is a Professor at the School of Chemistry at the University of New South Wales (UNSW), and the head of UNSW Nanoelectrochemistry Lab of ~30 researchers. He is also a Professorial Future Fellowship from Australian Research Council. He currently is the Chair of the Royal Australian Chemical Institute (RACI) Electrochemistry Division, and elected the Fellow of Royal Society of Chemistry (FRSC), Fellow of RACI (FRACI) and Fellow of Royal Society of New South Wales (FRSN). Prof Zhao received his PhD in 2002 with an excellence award from Northwest University, then completed postdoctoral research at University of Oldenburg and Monash University. He started his independent research career as a Lecturer at UNSW in Oct 2010, and was promoted to full Professor in 2017. Prof Zhao's research focuses on discovering novel electrochemical methods, nanomaterials and ionic liquids and their implications to electrochemical energy storage and conversion, and sensors applications including hydrogen production from water splitting, hydrogen fuel cells, CO₂ reduction, ammonia synthesis, and batteries.

Christian Zuluaga-Bedoya

Transport of light gases across single-crystal zeolite (MOF) nanomembranes: effect of size, flexibility, and polymer coating

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Zeolite (MOF) nanomembranes exhibit high separation performances due to their molecular sieving effect associated with precisely sized pores and tuneable frameworks, which makes them attractive for gas separation, carbon capture, and water treatment, among other applications [1]. Although pore characteristics of zeolites (MOFs) are well-defined, challenges pertaining to gas transport resistances within nanosized crystals remain unexplained. Empirical studies linked these transport hindrances to defects within the crystal formation process, resulting in pore obstructions and grain boundaries [2]. However, recent simulation-based investigations have uncovered nonuniform diffusivities and transport resistances persist even in nanometric-sized crystals with ideal surfaces. Although these resistances were initially ascribed to interfacial effects on the boundary layer [3], recent simulations attribute them to slow trajectories and an increased number of collisions within a region of developing flow known as entry length [4].

We study the effect of crystal thickness and framework flexibility on gas diffusion, by comparing a fully flexible system with a rigid-average structure of equivalent window size. Equilibrium Molecular Dynamics (EMD) simulations were used to study the transport of CO₂ in ZIF-8 and CH₄, H₂ in TON nanosheets of different sizes. We also investigated adding polymer layers (6FDA-durene polyimide) on TON bare nanosheets to account for support/both-side coating effects on the excess resistance. Transport is attenuated even in flexible thin nanosheets, despite having enhanced diffusivities compared to the rigid ones. An interplay between vibrating windows and kinetic effects on gas-wall collisions leads to increased diffusivity. Incorporating polymer layers into the nanosheets added extra internal barriers. Ideal selectivity is superior in the coated/supported at a particular crystal length. These results will aid in a better understanding of the transport resistances, guiding the fundamental design of ultrathin membranes for emerging sustainable applications.

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Biography



Christian Zuluaga-Bedoya is a current PhD candidate from the School of Chemical Engineering under the supervision of Prof. Suresh Bhatia. He obtained his Master's and Bachelors' degree in Chemical Engineering from the National University of Colombia, in process modelling and dynamic properties. He joined Prof. Suresh Bhatia's group in 2019 as PhD student, where he is studying the surface barriers using Equilibrium Molecular Dynamics.

Colin A. Scholes

Carbon dioxide hydrogenation to methanol through CuO/ZrO₂-polymer composite membrane reactor.

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Methanol is an excellent hydrogen carrier due to its high energy density as well as being a crucial precursor chemical for many industrial applications. The conventional method for methanol synthesis is via syngas from natural gas, but this approach has a large carbon footprint. Methanol can alternatively be synthesized by the carbon dioxide hydrogenation reaction, which represents a strategy to mitigate carbon emissions. However, the conversion of carbon dioxide to methanol faces challenges due to both thermodynamic restrictions and catalyst deactivation induced by the by-product water. To address these challenges, this research focused on the development of a novel catalytic membrane reactor based on flexible polyimide-based membranes. These membranes are selective for methanol at high temperature, enabling the products (methanol and water) to be separated from the reaction in-situ and hence overcome the thermodynamic limitation. The catalyst was based on nanostructured CuO/ZrO₂ thin films deposited on the polymeric membrane surface through novel methods. This ensured the catalyst interacted directly with carbon dioxide and hydrogen, rather than being imbedded within the membrane layer where catalytic interactions are restricted. Under operating conditions of 200 °C and 20 bar, the catalytic membrane reactor exhibits exceptional performance, achieving a significantly higher carbon dioxide conversion rate and methanol selectivity compared to a conventional catalytic fixed bed reactor. Hence, this membrane reactor design enables methanol synthesis from carbon dioxide to be a viable route for the synthesis of this important precursor chemical while reducing carbon emissions.

Biography



Colin A. Scholes CChem FRACI CEng MIChemE is an Associate Professor in the Department of Chemical Engineering at the University of Melbourne. He is an expert in clean energy processing and membrane science, particularly developing technologies to capture carbon emissions and assist the transition to low carbon hydrogen based fuels.

Dae-Hyun Nam

Metallurgical Alloy Electrocatalysts for Selective CO₂-to-Ethylene/Ethanol Conversion

Dae-Hyun Nam

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Electrochemical CO₂ Reduction reaction (CO₂RR), which converts CO₂ into value-added fuels and chemical feedstocks, offers an avenue toward carbon neutrality. At the heart of this reaction is the heterogeneous catalyst, a material which activates substrate species, induces proton/electron transfer, and interacts with reaction intermediates. For selective conversion of CO₂-to-multi-carbon (C₂₊) chemicals such as hydrocarbons and oxygenates, judiciously controlled Cu-based electrocatalysts which enable *CO dimerization for C-C coupling are required. To control the selectivity between ethylene (C₂H₄) and ethanol (C₂H₅OH), metal alloy has received great attention to tune the d-band center and induce spillover effect. Steering CO₂RR pathways for selective C₂H₄ and C₂H₅OH production is being studied; yet it remains a challenge to optimize the selectivity and productivity.

In this talk, I will present our recent efforts to address these challenges by metallurgy-based material design for CO₂RR heterogeneous electrocatalysts. We develop 'Nano-Metallurgy', a thermodynamic-based nanomaterial design principle to understand and predict the material phenomena in the catalyst fabrication and reconstruction during CO₂RR. This enables the predictive synthesis of nanomaterials by providing the processing window for selective oxidation/reduction of the elemental components. By applying this fundamental to alloying/dealloying process, we introduce how we control the interface of Cu-Ag alloys beyond miscibility limits for efficient selectivity control between C₂H₄ and C₂H₅OH. Also, in terms of atomic miscibility and oxidation tendencies, we elucidate how this principle can be applied to understand the Cu alloy reconstruction which changes the phase and structure of metallic species during CO₂RR.

Biography



Dae-Hyun received B.S. degree (2011) and Ph.D. degree (2017) from Department of Materials Science and Engineering, Seoul National University, Republic of Korea (Supervisor: Prof. Young-Chang Joo). He worked as postdoctoral fellow in Department of Electrical and Computer Engineering, University of Toronto, Canada (Supervisor: Edward H. Sargent) from Sep. 2017 to Jan. 2020. Since Feb. 2020, he is working as Assistant professor in the Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Republic of Korea.

Daksh Shah

TiO₂/CoAl-LDH nanocomposites for CO₂ photoreduction

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It is anticipated by 2040 that global energy demand will increase by 28%, at current emission rates, CO₂ levels will reach up to 750 ppm by 2050. This will increase average global temperatures by 2.7 °C [1]. Sunlight is the most abundant renewable energy source on Earth, providing 100000 TW per annum, exceeding annual global energy consumption [2], and hence offers a means to transitioning away from reliance on fossil fuels. Mimicking biological photosynthesis, inorganic semiconductors can be harvest light energy to enable charge separation, and thereby drive the photocatalytic reduction of CO₂ to hydrocarbons [3].

One of the key steps to realize CO₂ photoreduction is the design of suitable semiconductors. Herein, we report the synthesis of TiO₂/CoAl-LDH, the nanocomposite semiconductors. By tuning the structure and morphology of the two semiconductor materials, the valence and conduction bands of the materials were adjusted to form heterojunctions in the structure. As such, the energy bandgap and light absorption region of the composite materials were modified, which would lead the CO₂ photoreduction towards the selectivity of methane. XPS was used to confirm the formation of the heterojunction. UV-Vis was employed to interpolate the band gap information, PL was used to study the lifetime of the charge carriers, and the work function measurements conducted by PESA. CO₂ photoreduction on these synthesized composite materials under UV and visible light conditions were conducted to examine the photocatalytic activities of the developed materials and to see how their photoreduction performance was correlated with their photoelectronic properties. It was found that low loadings of LDH onto TiO₂ nanostructures boosted their selectivity towards methane by as far as three times the pristine counterparts. This was due to the successful construction of a nanocomposite material, with high surface area, basicity, and formation of a heterojunction with complimentary band gaps.

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Biography

Daksh Shah is a chemical engineer and a final year PhD candidate at RMIT University, studying inorganic semiconductor materials for solar fuels generation in collaboration with CSIRO. He is passionate about designing, engineering, and testing green materials for environmental remediation.

David Winkler

Artificial Intelligence for Materials Sciences, Quo Vadis?

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The current era has seen some paradigm shifting scientific developments, especially in big data and machine learning. It is now also widely understood that the size of small molecule and materials spaces is essentially infinite, providing scope for finding bespoke materials with greatly improved properties for diverse applications.

The need to find 'islands of chemical utility' in this vast palette of possibilities, and to extract meaning from massive datasets, has seen an impressive rise in both applications of AI and data driven machine learning, and development of new machine learning methods. There has been a parallel rise in their applications to most aspects of modern life, such as medicine, finance, manufacturing, social media etc. Recently, we have seen the development of rapid and accurate quantum machine learning methods, the use of generative methods that use trained machine learning models to suggest new molecules or materials with improved properties, accurate prediction of protein structures from sequence, the beginning of general AI in ChatGPT and variants, the availability of massive (>30B) 'make on demand' chemical libraries, the first experiments in autonomous chemical discovery systems with no human in the loop, and the increasing use of other AI methods (evolutionary algorithms) to discover molecules and materials with improved properties.

This presentation will discuss progress in these developments, describe some of the pitfalls encountered, summarize the contribution my collaborators and I in adapting and applying machine learning over the past three decades, and provide examples of applications to materials for environmental and energy gas storage and conversion.

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Biography



David Winkler is Professor of Biochemistry and Chemistry at La Trobe University, Professor of Pharmacy at the University of Nottingham, and Professor of Medicinal Chemistry at Monash University. He applies computational chemistry, AI, and machine learning to the design of drugs, agrochemicals, electrooptic materials, nanomaterials, green corrosion inhibitors, catalysts, and biomaterials. He is a recipient of an ACS Skolnik award, an RACI Distinguished Fellowship and Adrien Albert award, and the AMMA Medal 2023. He has written >300 journal articles and book chapters (5 ISI Highly Cited) and is an inventor on 25 patents.

Debra Bernhardt

Contributions of Simulation to Green Transformation of Carbon Dioxide

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Computation has become an important tool in development of clean technologies. For electrolytic conversion of CO₂, there are many aspects that can benefit from understanding and predictions enabled through computation. These span all levels from the atomic level where electronic structures can be explored to bulk scale where computational fluid dynamics is required, and everything between. Computation can be used to explore reaction mechanisms, catalysts, and interfaces as well as molecular transport, heat flow and conductivity. Tuning of fields, temperature and pressure can be modelled and structural features from the nanoscale to bulk scale are relevant. Multiscale modelling, machine learning and the integration of computation with laboratory experiments are necessary to enable some problems to be solved. With such a range of possibilities, careful selection of the best questions to address becomes important. In this talk I will discuss some of the challenges and opportunities for research in this area.

Biography



Debra Bernhardt is an ARC Australian Laureate Fellow in the Australian Institute for Bioengineering and Nanotechnology (AIBN) and School of Chemistry and Molecular Biosciences (SCMB) at The University of Queensland. Her research program focuses on theoretical and computational approaches to develop a fundamental understanding of the behaviour of matter. She applies these approaches to a wide range of problems, particularly transport in nanoscale systems, nonequilibrium flow, design of materials, energy storage and conversion. She is a Fellow of the Royal Australian Chemical Institute and Fellow of the Australian Academy of Sciences. Debra publishes as Debra J. Searles.

Fangzhou Liu

Understanding the Degradation Mechanism of Iron Phthalocyanine- for Acidic Oxygen Reduction Reaction

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Atomically dispersed iron (Fe) and nitrogen (N) co-doped carbon (M-N-C) catalysts show one of the best catalytic activities among platinum group metal-free catalysts for oxygen reduction reaction (ORR) in acidic conditions. They also have potential applications in the electrochemical reduction of CO₂. However, their critical problem is their poor stability. M-N-C catalysts synthesized via high-temperature methods lack control over their atomic structures to provide a clear understanding of their stability. Here, we design heterogeneous molecular catalysts by anchoring molecular structure-defined iron phthalocyanine (FePc) molecules on carbon nanotubes to resemble catalytically active sites in M-N-C catalysts. Hydrogen atoms in the four phenylene groups of FePc are replaced by various substituents (R) to alter their molecular structures, which change their catalytic activity and stability. We compare the degradation of a series of such catalysts in ORR under acidic conditions and quantify the contributions from different degradation paths, including FePc Desorption, Fe Leaching, FeO_x formation and so on. We show that the performance decrease of iron single-atom catalysts under acidic conditions mainly comes from the metal active site leaching. However, in the early stages of stability testing, iron will appear near the catalyst in the form of FeO_x and gradually leach over time, the previous method of evaluating catalyst stability based solely on the iron ion content in the electrolyte has certain limitations. Our findings provide a better understanding of the degradation mechanisms of M-N-C catalysts and pave the way to improve their stability for practical applications.

Biography



Fangzhou Liu is a Ph.D. student supervised by Prof. Yuan Chen and Dr. Li Wei at The University of Sydney. His research focuses on catalyst design and degradation mechanisms in acidic ORR.

Feng Jiao

CO₂ Electrolysis Systems for Chemical and Food Production

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As our society faces the pressing challenges of climate change and global warming, driven in part by increasing atmospheric CO₂ levels, reducing CO₂ emissions has become a critical mission in the pursuit of a sustainable future. Traditional chemical industry processes often rely on fossil fuels, which inevitably emit substantial quantities of CO₂. In response, electrochemical processes have garnered interest for their potential to be more environmentally friendly and exhibit a smaller carbon footprint when powered by renewable energy sources. Our research group is currently dedicated to the development of CO₂ electrolysis devices that convert CO₂ into value-added chemicals and fuels through innovative electrocatalyst design and reactor engineering. In this presentation, we will showcase our recent work on a two-step tandem CO₂ electrolysis system. We have reported an internally coupled purification strategy that significantly enhances acetate concentration and purity in CO electrolysis.[1] This approach employs an alkaline-stable anion exchange membrane with high ethanol permeability and a selective ethanol partial oxidation anode to regulate the CO reduction product stream. We successfully demonstrated a stable 120-hour continuous operation of the CO electrolyzer at a current density of 200 mA cm⁻² and a full-cell potential of less than 2.3 V, consistently producing a 1.9 M acetate product stream with a purity of 97.7%. This performance is among the best reported in the literature. The ability to convert CO₂ into acetate has opened the possibility of developing an electrochemical-biological hybrid approach to produce food from CO₂, offering much higher efficiency than natural photosynthetic pathways.[2]

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Biography



Professor Feng Jiao holds a BSc in Chemistry from Fudan University in China and a PhD in Chemistry from the University of St Andrews in the United Kingdom. Following the completion of his postdoctoral training at the Lawrence Berkeley National Laboratory, he joined the faculty at the University of Delaware in 2010. Then, he was promoted to full professor in 2021 and served as the Director of the Center for Catalytic Science & Technology. In August 2023, Professor Jiao joined the Department of Energy, Environmental & Chemical Engineering at Washington University in St. Louis as the Elvera and William R. Stuckenberg Professor. He also serves as the founding director of the Center for Carbon Management. The Jiao research group is developing innovative electrochemical devices to address critical energy and sustainability challenges. Professor Jiao has published over 100 research papers, which have collectively received more than 17,000 citations. His contributions have been recognized with several awards and honors, including his election as a Fellow of the Royal Society of Chemistry, the receipt of the NSF CAREER Award, and recognitions as a 2020 Emerging Investigator by the *Journal of Materials Chemistry A* and a 2020 Scialog Fellow for the Negative Emission Science (NES) initiative.

Fengtao Fan

Spatiotemporal imaging of charge transfer in photocatalyst particles

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Understanding the charge separation mechanism at the spatiotemporal scale is the core scientific problem in solar energy conversion, yet it is highly challenging. Focusing on this crucial point, we developed the surface photovoltage microscopic method with high spatial resolution. With this method, the charge distribution on the photocatalytic particle was quantitatively studied at the nm/ μm scale. Moreover, the vector addition effect of the built-in electric field on efficient charge separation has been revealed. On the basis of the above understanding, electric field management through asymmetric tuning strategies was proposed to align the electric field to the catalytic reaction site precisely, resulting in improved photocatalytic performances. Furthermore, spatiotemporally resolved surface photovoltage (SPV) techniques were developed to map charge transfer processes holistically from the femtosecond to second time scale at the single-particle level. New processes of ultrafast hot electron transfer and anisotropic trapping regimes were found, challenging the classical model and contributing to efficient charge separation in photocatalysis. These findings pave the way for the rational design of photocatalysts with improved performance.

Keywords: photocatalysis; charge transfer; imaging; spatiotemporal

Biography



Fengtao Fan is a Chair Professor at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences. He is a Distinguished Young Scholar of NSF of China and Fellow of the Royal Society of Chemistry. Currently, he serves as the Vice-Director of the State Key Laboratory of Catalysis, Secretary-General of the Catalysis Division of the Chinese Chemical Society, and Associate Editor of ChemComm.

His research focuses on heterogeneous catalysis, photocatalysis and electrocatalysis, with a particular emphasis on understanding the fundamentals of these processes using advanced space- and time-resolved spectroscopy. He has published over 100 papers in renowned international journals such as Nature, Nature Energy, Nature Commun., Natl. Sci. Rev., J. Am. Chem. Soc. Angew Chem.

Francis McCallum

Enhancing the Durability of Polymeric Materials via Sequential Infiltration Synthesis

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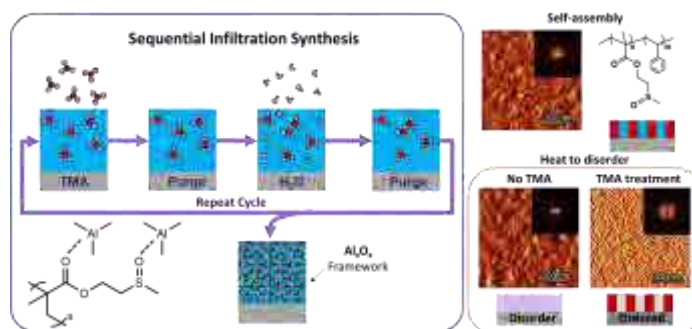
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Electrolyser membranes have the potential to play an essential role in capturing atmospheric CO₂ for conversion into valuable products. However, the materials traditionally used for these membranes often lack the robustness to withstand high thermal and mechanical stresses.¹ In this study, we explore the potential of Sequential Infiltration Synthesis (SIS) as a solution to this challenge. Initially developed for photolithography applications, SIS enhances ultra-thin polymeric films' mechanical and thermal stability by infiltrating metal oxide precursors into the free-volume. We investigated the Lewis acid/base interactions between trimethylaluminum (TMA) and poly(methyl methacrylate) (PMMA) using NMR and liquid cell transmission FTIR. We also introduced a novel SIS-compatible polymer, poly((2-methylsulfinyl) ethyl methacrylate) (PMSEMA), which incorporates a stronger Lewis base group, sulfinyl. Our work shows that PMSEMA has great potential to broaden the current SIS polymer library and meet current material hardening challenges in lithography. Moreover, we demonstrate that SIS significantly improves the thermal stability of nanostructures generated from the self-assembly of block copolymer PMSEMA-*b*-PS with covalently attached polystyrene (PS). While SIS has been primarily employed in lithography, our findings suggest its promising applicability in enhancing polymeric membrane mechanical and thermal properties in CO₂ reduction.



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Biography



Francis earned his Bachelor of Biotechnology with a Major in Nanotechnology in 2019, graduating with first-class honours from the University of Queensland. His honours research focused on the design and synthesis of high χ galactose-based block copolymers aimed at advancing materials for nanolithography. In 2020, he began his doctoral studies at the Australian Institute for Bioengineering and Nanotechnology (AIBN) as part of the Whittaker Group. Francis's current PhD research focuses on developing novel polymers optimised for Sequential Infiltration Synthesis (SIS).

Gang Kevin Li

In-situ vapor promoted direct air CO₂ capture

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Direct Air Capture (DAC), a groundbreaking concept in the realm of climate solutions, has emerged as a pivotal avenue for achieving negative emissions. By directly extracting CO₂ from ambient air, DAC offers a unique advantage by addressing the root cause of increasing atmospheric CO₂ levels. Among DAC methodologies, the adsorption-desorption process utilizing solid adsorbents presents notable promise. However, the large heat of adsorption requires high energy consumption for regeneration of adsorbents, significantly compromising the economic viability and productivity of DAC.

Here, we show a vapor promoted DAC process to recover the adsorbed CO₂ by in situ vapor purge using water harvested from atmosphere synergistically. The desorption of CO₂ is substantially enhanced in the presence of concentrated water vapors at around 100 °C, resulting in the concurrent production of 97.7% purity CO₂ and fresh water without the use of vacuum pumps. Moreover, we demonstrate a prototype of this DAC powered by sunlight, which recovers 98% of the adsorbed CO₂, the highest among all other DAC technologies, and consumes 20% less thermal energy. In another case when 10 kPa vacuum is applied, this in situ vapor purge can achieve near complete regeneration of the chemisorbents at temperatures as low as 60 °C, producing 99% purity CO₂ with a stable working capacity of 1.10-1.13 mmol/g for 45 cycles. The minimum work required for regeneration was only 1.62 MJ/kgCO₂, over 37% lower than temperature-vacuum swing desorption. This low-temperature regeneration process not only reduces the exergy demand but also reduces the overall cost of DAC.

Biography



Gang Kevin Li is an associate professor at the Department of Chemical Engineering, the University of Melbourne. He obtained his PhD in pressure swing adsorption technologies from Monash University. He is the chief investigator of the Clean Energy Laboratory, and a research theme leader of the ARC Centre for LNG Futures. Kevin is specialized in the areas of CO₂ capture and reduction, hydrogen production, enrichment of coal bed methane, and natural gas processing. He has more than 130 journal publications including *Nature*, *Nature Communications*, *Journal of the American Chemical Society*, *AIChE Journal*, and etc, and over 30 patents. His research has led to multiple spin-out companies and attracted over \$12M investment fund from leading industry partners, governments, and venture capitals such as Breakthrough Energy Ventures. He received the ARC DECRA in 2013, Western Australia Innovator Of The Year (2015), ExxonMobil Award of Excellence in Chemical Engineering (2019), and the ATSE David and Valerie Solomon Prize (2020).

Geoff Wang

Development of Technologies Approaching to Low Emission and Carbon Neutrality for Steel Industry

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Ironmaking and steelmaking are energy intensive processes that significantly contribute to the CO₂ emissions, estimated at 1.85 tonnes of CO₂ emissions per tonne of steel produced from a conventional blast furnace (BF) - Basic Oxygen Furnace (BOF) route. More than 70% of these CO₂ emissions are resulted from the ironmaking BFs. Therefore, developing the low-carbon ironmaking technology to reduce the CO₂ emissions of the BF-BOF process is a significant challenge in the sustainability of iron and steelmaking. This talk briefings our recent research in low-carbon ironmaking and discusses the CO₂ capture and utilization opportunities in ironmaking process with a feasibility study on the alternative BF top gas recycling by means of CO₂ capture and CO₂ electrochemical conversion. As a result, a CO₂-to-CO electrolysis process integrated ironmaking technology is proposed, which could significantly reduce coke consumption in BF and realize up to a 42% reduction in the CO₂ emissions per tonne of steel due to the carbon recycling.

Biography

Professor Geoff Wang received his PhD in Metallurgical Engineering (Ironmaking and Steelmaking) from the Northeastern University, Shenyang, China in 1990, and then worked in Wuhan University of Science and Technology for 5 years and then about 2 years at University of New South Wales. He joined the University of Queensland in end of 1996 until now. His research activity and interests are directed towards developing energy and environmental technologies dealing with the coal and steel industries. He has been active and performed the research programs in clean energy and low-carbon technologies such as pulverized coal injection into blast furnaces, modelling in ironmaking and steelmaking, hydrogen production through lower emission coal combustion, coal seam gas recovery and CO₂ sequestration, and in recent years, the chemical and electrochemical conversion of CO₂ to fuel or reusable chemicals and carbon recycling in ironmaking blast furnace.

Gloria Monsalve

Gas sorption isotherms in glassy polymer membranes: are mixture predictions sensitive to parameter uncertainty?

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Investigation of mixed-gas sorption is necessary for robust design and optimization of membrane-based processes. While sorption models for glassy polymers are well-established, they often deviate from observed mixture data. In doing so, however, parameters of these models are typically estimated via traditional least-squares optimization methods, and so parametric uncertainty is often ignored in mixture sorption predictions. As an alternative, we use Bayesian Inference (BI) to estimate probability distributions for sorption models' parameters and thus provide statistically meaningful mixture sorption forecasts that reflect parameter uncertainty rigorously. To this end, we exploit molecular sorption simulations, combining Grand Canonical Monte Carlo (GCMC) and Equilibrium Molecular Dynamics (EMD), to focus on two different glassy polymer systems (i.e., single- and mixed-gas sorption of CO_2/CH_4 in a fluorinated polyimide and CH_4/H_2 in a polymer of intrinsic microporosity) and three popular mixture sorption models (the Dual-Mode Sorption model, Non-Equilibrium Thermodynamics for Glassy Polymers model, and the Ideal Adsorbed Solution Theory) to demonstrate the benefits of this technique for uncertainty quantification and propagation in membrane applications. We show that observed sorption data at typical working pressures (e.g., 0–25 atm) are often insufficient to accurately estimate model parameters, and consequently, these models often fail to adequately represent observed mixture data. Furthermore, we show that sorption data (e.g., high-pressure data), able to capture intrinsic isotherm nonlinearities of sorption models, are critical to considerably improve parameter inference from collective model-data fits and thus accurately predict mixture sorption.

Biography



Gloria is an Advance Queensland Industry Research Fellow at The University of Queensland's School of Chemical Engineering, where She uses novel multiscale simulation techniques, combining molecular simulations with macroscopic physics-based modeling, to solve energy and environmental problems. She works at the interface between applied mathematics and engineering to build models to explore and improve understanding of phenomena driving behaviour of complex systems as well as to develop computational methods to improve simulation tools for multiple applications, ranging from chemical and biomedical engineering to ecology.

Graeme Henkelman

Correlating structure and function for nanoparticle catalysts

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In this talk I will discuss our efforts to model the structure of metal nanoparticles how they function as catalysts for small-molecule reactions. In many cases we are able to successfully generate a model for the forward problem, where we have a known structure and determine the catalytic function that is consistent with experiment. More challenging is the inverse problem where we try to predict the structure of a new catalyst with a desired catalytic function. I will show, with examples, that in some cases catalytic properties change smoothly with structure and our predictions are validated experimentally. In other cases, the theoretical predictions fail, and that can lead to equally interesting outcomes through the process of finding agreement between theory and experiment.

Biography



Graeme Henkelman is a professor of chemistry at the University of Texas at Austin. He did his undergraduate work in physics at Queen's University in Canada, a PhD in chemistry at the University of Washington in 2001, and a postdoc at Los Alamos National Lab before starting at UT in 2004. His research group has focused on computational methods for modeling reaction dynamics over experimental time scales. These methods are applied to the challenge of developing new materials for energy applications including catalysts and batteries.

Graeme Puxty

Aromatic amines for CO₂ capture applications

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Over the past few decades a great deal of research effort has been brought to bear on developing amine based CO₂ absorbents with improved performance characteristics relative to aqueous monoethanolamine (MEA). The important performance characteristics are the energy required for CO₂ desorption, rates of mass transfer, long term stability in the presence of O₂ and high temperatures, corrosion, volatility, toxicity and biodegradability. To-date the focus has been on aliphatic molecules and absorbent formulation. For example aqueous blends of 2-amino-2-methyl-1-propanol (AMP) and piperazine (PZ) are probably the best known absorbent formulations that yield benefits relative to MEA across most of these characteristics [1-2].

Aromatic compounds have received little attention as potential CO₂ absorbents, most likely due to their assumed low aqueous solubility and toxicity (think polyaromatic hydrocarbons). They are also inherently stable and often associated with persistent organic pollutants. However, the addition of heteroatom functionality such as amino groups alters many of these properties in a favourable way, while retaining greater stability than aliphatic compounds. Our research has found that aromatic amines uniquely combine multiple properties favourable for CO₂ capture applications [3]. Of note is a low energy requirement for CO₂ desorption and enhanced stability when exposed to oxygen and thermal cycling. The low energy requirement is a consequence of a highly rigid aromatic ring structure resulting in a small or even negative entropy change upon protonation of associated amino groups. Similarly, the enhanced stability results from the highly stable aromatic structure, that when degradation does occur, results in formation of a single product that can be extracted and recycled. These features combined make for a unique absorbent dubbed CAL008 that has been demonstrated at pilot scale in multiple flue gas environments. This presentation will describe the development of our aromatic amine based CAL008 absorbent and its performance.

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Biography



Graeme studied chemistry and computer science at The University of Newcastle (AU) and completed his PhD in Chemistry in 2004. In 2007 Graeme joined CSIRO and is currently a Principal Research Scientist and Team Leader in the Sustainable Carbon Technologies Group. Graeme has published over 100 journal articles, 5 book chapters and holds 7 patents. He is also a Frontiers in Energy Research Associate Editor and an expert reviewer for the GHGT conference series. His research has focused on the chemical and physical processes involved in the separation of carbon dioxide and other acid gases from gas mixtures, and their potential transformation into valuable materials.

Hai Yu

Integrated carbon capture and utilization for sustainable carbon mining

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CSIRO is recognized internationally for its expertise in liquid absorbents based, CO₂ capture technology. CSIRO and its industry partners designed, built, and operated three pilot plants in Australia to develop, assess and advance carbon capture technologies under real flue gas conditions. Intensive and collaborative research has led to the development of an advanced liquid absorbent, CAL008 that demonstrated outstanding performances at pilot plant scale in Australia and USA. Currently we are commercializing the CAL008 based capture technology with our partners. Recently we have extended our research to direct air capture and CO₂ utilization to make low emission materials including fuels, chemicals, and construction materials. This talk will briefly present our research progress in these areas, including:

- (1) CAL008 capture absorbent development. 5000 hour trial with CAL008 at AGL Loy Yang Power Station has showed significant improvement over commercially available absorbents: Amine formulation not affected by NO_x; Achievable reboiler duty: < 2.5 GJ/t CO₂ with optimised process design; Amine consumption: < 0.3 kg/t CO₂; Biodegradable and low toxicity.
- (2) Integrated capture and conversion. Through direct mineralization or electrolysis of the captured CO₂ in aqueous solution, the novel processes are under development: Integrated absorption and mineralization (IAM) to make construction materials from CO₂ and alkaline solid wastes, two birds one stone; Integrated capture and electrolysis (ICE) to enable low-cost production of renewable materials from CO₂ and water. The new processes potentially eliminate energy intensive regeneration steps, allowing production of low emission products in a simple, cost-effective manner, supporting a new industry, sustainable carbon mining and a circular economy.

Biography



Dr Hai Yu is a principal research scientist and a team leader with CSIRO Energy. His research covers both fundamental and applied aspects of CO₂ capture, multiple pollutant removal, integrated carbon capture and mineralization, conversion of greenhouse gases to value added chemicals/fuels, and process simulation and optimization, and technical assessment. Currently he is leading a team to develop a roadmap for carbon capture, utilisation and storage for production of low emission cement and lime in Australia. Through broad and deep collaboration within CSIRO and Australian universities and industry, he has been developing innovative, integrated capture and conversion technologies which potentially eliminate energy intensive regeneration steps and enable production of low emission products in a simple, cost-effective manner, supporting a new industry, sustainable carbon mining and a circular economy.

Hao Li

The *Cat*-Universe: A “Data-Theory-Methodology-Experiment” Framework to Realize Catalyst Design

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The design of solid-state materials is essential for a sustainable future. However, conventional materials search relies on the trial-and-error process from experiments. Meanwhile, theoretical analysis of materials is sometimes too complicated to develop a clear guideline for experiments. This talk will discuss an avenue to realize a data-driven framework for materials design combining data-mining, materials theory, computational methodology development, and experiments. In particular, we will discuss i) how to reduce the complexity in catalyst design by materials theory and ii) how to develop new computational methods (*i.e.*, new package, model, and algorithm) to accelerate materials simulation. This talk will show the predictive power of theory in electrochemical and thermal catalysis, solid-state electrolytes, and hydrogen storage materials. We will also discuss the successful design of an “electron-refinery” strategy by transforming high-temperature thermal catalysis into low-temperature electrocatalysis. Finally, we will discuss the practical design of materials (in particular, for CO₂ conversion) combining data science, materials theory, computational screening, computational methodology development, and experiments.

Reference

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Biography



Hao Li is an Associate Professor at the Advanced Institute for Materials Research (WPI-AIMR) of Tohoku University, Japan. He developed the “Digital Catalysis Lab (*DigCat*)” as the Principal Investigator in 2022. He obtained his Ph.D. degree at University of Texas at Austin. He was a postdoc researcher at Technical University of Denmark, in the group of Prof. Jens K. Nørskov. Hao’s research interests consist of i) development of materials and catalysis theory, ii) development of computational methodology based upon AI, and iii) design of cost-effective catalysts, batteries, and hydrogen storage materials with special emphasis on sustainable production. Since 2015, Hao has published >155 refereed articles in world-leading journals such as *Nature Catal.*, *Nature Comm.*, *JACS*, *Adv. Mater.*, *Energy & Environ. Sci.*, *Chem. Sci.*, and *ACS Catal.* He has received notable honors & awards, including: “Top 2% of the World’s Most Highly Cited Scientists” (Stanford & Elsevier, 2021 & 2022), “Surface Science Young Investigator” (ACS, 2022), “AIChE Best Fundamental Paper Award” (2020), and “Emerging Investigators in Materials Chemistry” (RSC, 2019). Since 2018, Hao has been invited to provide >40 public talks in leading universities and conferences, including Cambridge, Princeton, Purdue, UQ, USYD, ANU, U. Manchester, Tsinghua, USTC, ACS Meeting, and Gordon Conference.

Haoming Yu

Biomass-derived carbon-based catalysts for electrocatalytic CO₂ reduction

Haoming Yu¹, Jun Wang², and Jie Zhang³

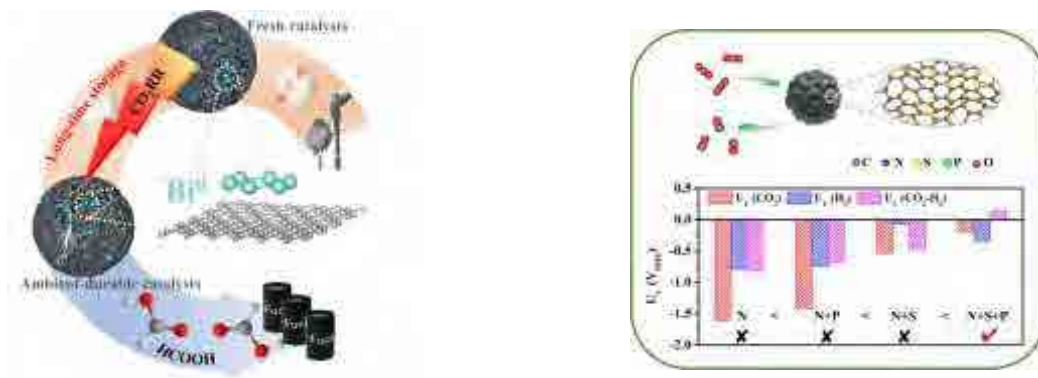
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Carbon materials are widely applied in electrocatalytic CO₂ reduction due to the advantages of high specific surface area, porosity, and electrical conductivity. We have used waste biomass as a carbon source to prepare carbon encapsulated metal catalysts and multi-heteroatom doped carbon catalysts by one-pot strategy. In this talk, I will present two of our recent works: 1. A carbon-encapsulated Bi nanocluster catalyst were synthesized using camphor seed as the carbon source. This catalyst achieved a FE_{HCOO⁻} of more than 90% over a wide potential range of 500 mV with a maximum FE_{HCOO⁻} of 96% at -1.15 V_{RHE}. Furthermore, the metallic Bi nanoparticle core was highly stable in air maintaining zero-valence in air for 30 days. The FE_{HCOO⁻} only decreased by 7.3%. 2. N, P, S co-doped carbon-based catalysts were prepared with waste shrimp shells as a carbon source and achieved a FE_{CO} of 92% at -0.7 V_{RHE} with an onset overpotential as low as 270 mV. It was demonstrated that multi-heteroatom co-doping resulted in the formation of an asymmetric electronic structure around the C atom thereby increasing the bonding strength to the *COOH intermediate and promoting CO formation. This study proposes an economical and green strategy to prepare high performance CO₂ reduction electrocatalysts from waste biomass, achieving the transformation of waste into treasure, consistent with the strategy of sustainable development.



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Haoxin Mai

Catalysts Synthesis and Development: What we can do for Electrochemical CO₂ Reduction

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With the intensification of human industrial activities, there has been a gradual disruption in the balance between CO₂ consumption and generation. This disruption has led to increased CO₂ production, heightening the urgency of global warming as a pressing concern. Therefore, it is imperative to reduce CO₂ emissions and explore methods for converting CO₂ into valuable materials to ensure a sustainable future. In recent years, electrochemical catalysis approaches for CO₂ conversion have attracted great attention.^[1] In contrast to thermodynamic methods, the electrochemical approach is considered environmentally friendly, utilizing sustainable electric energy from sources like wind or solar power. Various electrocatalysts, such as metals,^[2] oxides,^[3] phosphates,^[4] have been developed to enhance catalytic activity and stability during reactions. However, CO₂ electroreduction is still challenged by sluggish kinetics, low energy efficiency, and multiple electron pathways. Thus, there is an urgent need to design highly selective and active catalysts for CO₂ reduction. Drawing from our previous research,^[5,6] we propose that a combined approach involving material synthesis, theoretical calculations, and statistical modelling will facilitate the development of CO₂ electroreduction catalysts and provide deeper insights into their physical and chemical principles.

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Biography



Haoxin Mai received his MSc degree in Information Technology and Computer Science from the University of Technology Sydney, and PhD degree in Materials Chemistry from the Research School of Chemistry at the Australian National University in 2019. He has worked at the Royal Melbourne Institute of Technology (RMIT) University as a research assistant from 2019. His research interests include perovskite photocatalysis and photoluminescence, ferroelectric thin films, controllable synthesis of inorganic colloid nanocrystals and machine learning.

Hesamoddin Rabiee

Microtubular Gas-diffusion electrode for electrochemical CO₂ reduction reaction

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Electrochemical CO₂ reduction reaction (CO₂RR) requires gas diffusion electrodes (GDEs) for efficient mass transport¹. Regulating the rational wettability of GDEs plays a pivotal role to improve the efficiency of CO₂RR². Herein, we present a wettability regulation strategy that modulates the triple-phase reaction zone in the catalyst layer. This strategy was employed on hollow fiber GDEs with several advantages over conventional planar GDEs^{3,4}. Dual-layer hollow fiber GDEs were fabricated via coating Cu microtubular electrode with a layer of Bi-loaded carbon nanotubes (CNT-Bi thickness: 15 μm). After that, since the CNT layer is hydrophobic, the electrolyte penetration depth into the CNT-Bi layer was controlled by an electrooxidation step for up to 20 s at 2.0 V. This leads to the controlled oxidation of inner layers of CNT-Bi and making it hydrophilic. As observed via fluorescence confocal microscopy, the electrolyte penetration increased with electrooxidation, and for 20s treatment, the penetration depth was 15 μm, and the CNT-Bi layer was fully wetted. Thus, the electrolyte can block the Cu substrate pores, which are CO₂ diffusional pathways, and this is not desired. For 15s electrooxidation, around 12 μm of the CNT-Bi layer was wetted, therefore distinctive hydrophilic-hydrophobic regions could be created. Compared to other ex-situ methods, such as doping hydrophobic agent or plasma/thermal treatment, affecting the electrocatalysts/catalyst layer bulk, our strategy created hydrophilic-hydrophobic regions and resulted in facilitating the species transport, boosting triple-phase interface formation, and maximizing the active sites. This regulation strategy showed stable wettability during CO₂RR conditions. The electrode with the optimal wettability (15 s treatment) exhibited over 80% catalyst utilization and 4 times higher formate partial current density (~150 mA cm⁻² with FE_{formate}> 90%) compared to the untreated electrode, outperforming other GDEs used for CO₂RR to formate in similar electrolytes.

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Biography



Hesamoddin Rabiee accomplished his Ph.D. from the University of Queensland, in 2022 with the Dean's Commendation for research excellence. His Ph.D. delved into electrochemical CO₂ conversion, focusing on the innovative design of electrodes to facilitate the efficient production of value-added chemicals. He has to date published over 35 peer-reviewed journal papers, with >1800 citations. He is currently a research fellow at the University of Queensland working in diverse areas, encompassing gas electrocatalysis, especially CO₂ conversion, membrane separation, CO₂ capture, and desalination – all aimed at promoting greener solutions for the future.

Huazhen Chang | Rujing Zheng

2D materials used for CO₂ adsorption

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Carbon dioxide (CO₂) adsorption is an important means to combat CO₂ emissions from flue gas and atmosphere. In recent years, 2D materials have attracted wide attention due to their unique structure and excellent electron transfer properties. Compared to other dimensional materials, the high mechanical strength and thermal stability of 2D materials help to maintain the durability^[1], and the larger specific surface area allows more active sites to be exposed. These advantages have also led to the upsurge of research on 2D materials in the field of CO₂ adsorption.

This paper would like to introduce the basic structure and properties of 2D materials represented by graphene, layered double hydroxides (LDH), boron nitride (BN), carbon nitride (C₃N₄) and MoS₂ in CO₂ adsorption. and then summarizes the modification schemes to improve their CO₂ capture capacity and stability. (i) The adsorption of CO₂ by graphene and its derivatives is mainly a physical adsorption of van der Waals interaction, by adding defects or functional groups to the graphene surface, the affinity of CO₂ to the graphene surface can be increased; (ii) The advantages of LDH are its economy and stability, and the adsorption capacity can be improved by changing the internal structure of LDH, forming LDH composite materials or improving the surface alkalinity; (iii) BN has a unique structure. The interaction between CO₂ and BN can be improved through the modification of electron donating groups or metal elements;(iv) C₃N₄ has the characteristics of high nitrogen content, either mesoporous or functionalization of C₃N₄ can improve its CO₂ adsorption capacity; (v) The adsorption of CO₂ by MoS₂ can be enhanced by vacancy defect treatment and element doping. Finally, the challenges and development prospects of 2D materials in CO₂ capture are proposed, to provide references for the development of 2D materials.

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Biography



Rujing Zheng is currently a MA candidate at the College of Environment and Natural Resources, Renmin University of China. Her research interests include the fabrication and application of solid CO₂ adsorbents and the analysis for CO₂ capture mechanism study.

Huijun Zhao

Green Electrochemical Transformation of Carbon Dioxide: Challenges and Solutions

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The use of renewable electricity-powered electrocatalytic carbon dioxide reduction reactions to produce chemicals/fuels not only curbs greenhouse gas emissions but also reduces our reliance on the rapidly diminished petroleum resources. Despite remarkable scientific progress, economically-viable production of chemicals/fuels via carbon dioxide reduction reactions faces a number of formidable challenges, for instance, directly converting simple CO₂ into high value-added carbon products with least energy input, achieving high operational current density under the limited CO₂ solubility in aqueous electrolytes, and the scalable fabrication of highly stable cathodes.

This presentation intends to illustrate pressing practical issues in electrocatalytic carbon dioxide reduction reactions. Several of our recent research findings will be used to exemplify potentially applicable approaches to address practical challenges.

Biography



Prof. Huijun Zhao is the Funding Director of the Centre for Catalysis and Clean Energy at Griffith University, the elected Fellow of Australian Academy of Science (FAA) and the Australian Academy of Technological Sciences & Engineering (FTSE), Fellow of Royal Society of Chemistry (FRSC) and Fellow of the Royal Australian Chemical Institute (FRACI). He has extensive expertise in functional materials, energy conversion/storage, catalysis and sensing technologies, and has published over 550 refereed journal papers and gained 68 international patents within 8 world-wide patent families. One of his current research pursuits is to explore new ways to unlock the catalytic capabilities of nonprecious materials as high performance catalysts for important catalysis reactions.

Ibrahim Orhan

Accelerating prediction of CO₂ capture at low partial pressures in metal-organic frameworks using new machine learning descriptors

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Metal-Organic frameworks (MOFs) have been considered for various gas storage and separation applications. Theoretically, there are an infinite number of MOFs that can be created; however, a finite amount of resources are available to evaluate each one. Computational methods can be adapted to expedite the process of evaluation. In the context of CO₂ capture, this paper investigates the method of screening MOFs using machine learning trained on molecular simulation data. New descriptors are introduced to aid this process. Using all descriptors, it is shown that machine learning can predict the CO₂ adsorption, with an R² of above 0.9. The introduced Effective Point Charge (EPoCh) descriptors, which assign values to frameworks' partial charges based on the expected CO₂ uptake of an equivalent point charge in isolation, are shown to be the second most important group of descriptors, behind the Henry coefficient. Furthermore, the EPoCh descriptors are hundreds of thousands of times faster to obtain compared with the Henry coefficient, and they achieve similar results when identifying top candidates for CO₂ capture using pseudo-classification predictions.

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Biography



Ibrahim Baris "Barry" Orhan is a candidate for a PhD in Applied Chemistry in RMIT University's School of Science. He obtained his bachelor's in mechanical engineering from Northeastern University (Boston, MA) in 2018, along with a minor in industrial engineering. He went on to complete his master's degree in Sustainable Energy through RMIT University (Melbourne, VIC) in 2020. His current PhD project is titled "Accelerated Material Discovery Through Machine Learning for Gas Adsorption and Storage" and is supervised by Dr Aaron Thornton (CSIRO), Dr Ravichandar Babarao (RMIT), Dr Tu Le (RMIT). The project involves the development of machine learning models and novel methods of numerically describing the candidate materials.

Ingo Pinnau

Materials Design for Membrane-Based CO₂ Separations

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The membrane-based gas separation industry has grown significantly over the past two decades with an estimated annual market size of ~ 1-1.5 billion USD due to its continuous operation, small footprint and competitive cost compared to conventional unit operation processes¹. Major successful industrial applications include (i) nitrogen production from air, (ii) hydrogen recovery from various process streams, (iii) air dehydration and (iv) CO₂ removal from natural gas and biogas. In these applications only very few glassy polymeric membrane materials, e.g., polysulfone, polyimide, cellulose acetate, are in large-scale industrial use. To further expand the current application spectrum to include capture of carbon dioxide emissions from power plants using membrane technology is a highly demanding task, because of the massive feed flow rates and low CO₂ concentration of 10-15 vol%. Currently, the best performing membrane materials are based on rubbery polyethers. Importantly, these highly hydrophilic polymers are easily solution-processible and can be transformed into high-performance thin-film composite membranes with CO₂ permeance of > 1000 GPU and CO₂/N₂ selectivity of >50. In this presentation, basic materials design principles are highlighted for various applications involving CO₂, i.e., removal from flue gas, syngas and natural gas.

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Biography



Ingo Pinnau is Professor and Chair of the Chemical Engineering Program in the Physical Science and Engineering Division at KAUST. Prior to his appointment at KAUST, Professor Pinnau worked for 18 years as Director of Materials and Membrane Development at Membrane Technology and Research, Inc., Menlo Park, CA, in the United States. Prof. Pinnau has co-edited four books on membrane science, is the author of 200+ peer-reviewed publications, and holds 52 granted U.S. patents. He served twice as President of the North American Membrane Society and belongs to the Editorial Board of the Journal of Membrane Science and Applied Water Science. Prof. Pinnau holds various professional memberships and has received several national and international awards.

Jeffrey Harmer

Studying Catalytic Reactions using Electron Paramagnetic Resonance Spectroscopy

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Electron Paramagnetic Resonance (EPR) spectroscopy, in both pulse and continuous wave (CW) mode, is a powerful technique to characterise paramagnetic centres in molecules (unpaired electron centres found in e.g., radicals and metal centres). In this talk I will provide an overview of contemporary EPR pulse and continuous wave techniques used to investigate catalysis in a variety of systems. I will highlight several recent projects in our laboratory including understanding the charge and discharge process in sodium ion battery electrodes, metalloenzyme catalysis by MCR, and the process of formate oxidation to carbon dioxide (or the reverse reaction) as catalysed by dehydrogenase FdsABG which contains a Mo active site and a molecular wire comprised of Fe-S clusters to transport electrons between the site of oxidation and reduction [1].

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Biography



A/Prof Jeffrey Harmer developed his international standing in the field of Electron Paramagnetic Resonance (EPR) spectroscopy through posts at two world class EPR centres; the ETH Zürich (2000-7) and the University of Oxford (2007-13). He returned to Australia in 2013 to take up an ARC Future Fellow (Level II) at the University of Queensland, where he is currently the EPR Group Leader at the Centre for Advanced Imaging. Harmer's research has made major advances in the application of pulse and continuous wave (CW) EPR techniques to elucidate the structure, function and reactivity of paramagnetic centres in molecules and materials, with an emphasis on exploring catalysis carried out by paramagnetic centres.

Jennifer Wilcox

The Role of Carbon Capture in Meeting Net-Zero Carbon Goals

Dr Jennifer Wilcox

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President Biden has laid out a bold and ambitious goal of achieving net-zero carbon emissions in the U.S. by 2050. The pathway to that target includes cutting total greenhouse gas emissions in half by 2030 and eliminating them entirely from the Nation's electricity sector by 2035. Investment in technology research, design, development, and deployment (RDD&D) will be required to achieve the president's objectives, including investments in both carbon capture at point sources in addition to carbon dioxide removal approaches that target the accumulated pool of carbon in the atmosphere. Both will be required to achieve net-zero carbon emissions in time and they will require increased deployment in order to move down the cost curve. These efforts combined with effective policy will make these approaches economically viable. These approaches are critical and they must be deployed in parallel. Deployment of these technologies at the scale required will necessitate the use of resources including land, water, and in some cases, low-carbon energy, while ensuring the secure and reliable storage of carbon dioxide (CO₂) on a timescale that impacts climate. Therefore, CCS and CDR deployment must be implemented strategically in terms of regional goals and requirements. The Office of Fossil Energy and Carbon Management will play an important role in the transition to net-zero carbon emissions by reducing the environmental impacts of fossil energy production and use – and helping decarbonize other hard-to abate sectors – through investments in technology solutions including CCS, direct air capture, and the deployment of carbon capture technologies to produce low-carbon products and fuel, including hydrogen.

Biography



Jennifer Wilcox is the Presidential Distinguished Professor of Chemical Engineering and Energy Policy at the University of Pennsylvania and is currently on leave to serve as the Principal Deputy Assistant Secretary for the Office of Fossil Energy and Carbon Management at the Department of Energy. At Penn, she oversees the Clean Energy Conversions Lab. She was previously the James H. Manning Chaired Professor of Chemical Engineering at Worcester Polytechnic Institute. Having grown up in rural Maine, Wilcox has a profound respect and appreciation of nature, which permeates her work as she focuses on minimizing negative impacts of humankind on our natural environment. Wilcox's research takes aim at the nexus of energy and the environment, developing both mitigation and adaptation strategies to minimize negative climate impacts associated with society's dependence on fossil fuels. This work carefully examines the role of carbon management and opportunities therein that could assist in preventing 2° C warming by 2100. Carbon management includes a mix of technologies spanning from the direct removal of carbon dioxide from the atmosphere to its capture from industrial, utility-scale exhaust streams, followed by utilization or reliable storage of carbon dioxide on a timescale and magnitude that will have a positive impact on our current climate change crisis. She has served on a number of committees including the National Academy of Sciences and the American Physical Society to assess carbon capture methods and impacts on climate. She is currently a member of the Energy & Environmental Science Journal Editorial Board. She is the author of the first textbook on carbon capture and, most recently, the CDR Primer.

Jinshuo Zou

Size Effects of Ru Nanoparticles in Li-CO₂ Batteries

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Nowadays, the dominant sources of power heavily rely on the combustion of fossil fuels such as coal, oil, and natural gas. This dependence has led to a substantial increase in atmospheric CO₂ levels, amplifying the greenhouse effect and its consequences. Li-CO₂ batteries offer a promising solution by enabling the capture of CO₂ and its conversion into a valuable energy storage medium. Ru based catalysts are dominating catalysts for Li-CO₂ batteries because of the ultrahigh catalytic activity toward CO₂ related reaction. However, the relationship between size and activity of Ru at the nanoscale remains significantly unexplored in the field of Li-CO₂ batteries. Here, we synthesize a series of Ru nanoparticles ranging from ~1.09 to ~7.41 nm deposited on CNTs, aiming at investigating the size-dependent activity in Li-CO₂ batteries. The d band centre of Ru is identified upshifted toward the Femi level with the decrease of Ru size and small Ru has stronger interaction with intermediates and products. The binding energy of Li-O and C=O is relatively lowered on small Ru particles, confirming that the strong interaction between Ru and Li₂CO₃ weakens the stable structure of Li₂CO₃ and promote the decomposition during charge. The ultrasmall particles are easily covered by the aggregated Li₂CO₃ which causes poor cycling stability. Remarkably, the ~2.05 nm Ru exhibits the best performance with the smallest overpotential of 1.1V after 1900 h cycling, which significantly surpasses the performance of other Ru-based Li-CO₂ batteries. Our findings shed light on how the size of Ru nanoparticles influences the weakening bonds in Li₂CO₃, the promotion of decomposition, and the overall enhancement of Li-CO₂ battery performance.

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Biography



Dr Jinshuo Zou is a postdoc in The University of Adelaide, Australia. She obtained her PhD degree in Feb 2022 from University of Wollongong, Australia. Her research interests focus on electrode preparation and mechanism study of electrochemical CO₂ reduction and Li-CO₂ batteries.

Juan Bai

Anion-Modulated Generation of Defective Molybdenum Sites as Synergistic Active Centers for Durable Oxygen Evolution

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It is well known that electrocatalytic oxygen evolution reaction (OER) activities primarily depend on the active centers of electrocatalysts.¹ In some oxide electrocatalysts, high-valence metal sites (e.g., molybdenum oxide) are generally not the real active centers for electrocatalytic reactions, which is largely due to their undesired intermediate adsorption behaviors. As a proof-of-concept, molybdenum oxide catalysts are selected as a representative model, in which the intrinsic molybdenum sites are not the favorable active sites.² Via phosphorus-modulated defective engineering, the inactive molybdenum sites can be regenerated as synergistic active centers for promoting OER. By virtue of comprehensive comparison, it is revealed that the OER performance of oxide catalysts is highly associated with the phosphorus sites and the molybdenum/oxygen defects. Specifically, the optimal catalyst delivers an overpotential of 287 mV to achieve the current density of 10 mA cm⁻², accompanied by only 2% performance decay for continuous operation up to 50 h. It is expected that this work sheds light on the enrichment of metal active sites via activating inert metal sites on oxide catalysts for boosting electrocatalytic properties.

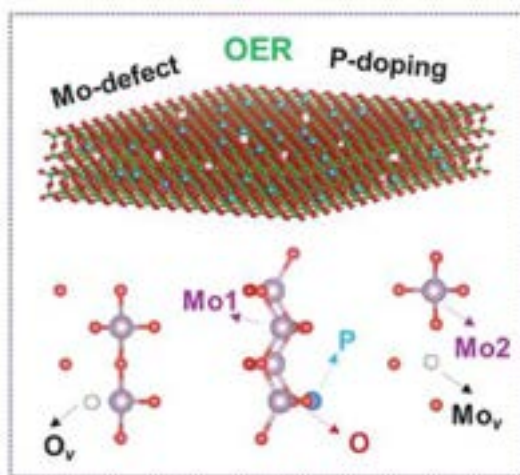


Figure 1. Schematic illustration of the catalyst models with the Mo-vacancy.

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Jun Chen

Defective carbon-based materials for electrocatalysis

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In the past few decades, tremendous efforts have been devoted to developing carbon-based materials to reduce the need for precious metals in the field of electrocatalysis.¹ Thereinto, defective carbon-based electrocatalysts have recently been considered one of the most promising alternatives owing to their irreplaceable advantages, such as environmentally friendly, low cost, and high structural tunability.²⁻⁴ However, despite remarkable progress has been achieved, grand challenges of their further development remain with the traditional “trial-and-error” approaches, mainly due to the lack of precise synthetic methodologies as well as in-depth understandings of active centres and underlying electrocatalytic mechanisms. Herein, we report some new synthetic strategies to precisely control the carbon defect density or manipulate the targeted migration of metal species on defective carbon substrate, which not only successfully realize the monitoring the structural dynamic evolution of DCMs, but also improve the fundamental understanding of the synthetic and electrocatalytic mechanisms. We believe that the development of synthetic methodologies of DCMs provides plenty of room for expanding the “gene pool” of electrocatalysts and then pushing the DCMs towards industrialization.

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Biography



Professor Jun Chen is currently appointed as Associate Dean of Australian Institute for Innovative Materials (AIIM), and Head of Postgraduate Studies of Intelligent Polymer Research Institute (IPRI), University of Wollongong (UOW). His research interests include: Electroactive Materials, Electro-/Bio- Interfaces, Nano/Micro- Materials, 2D/3D Printing and Wearable Electronic Devices. Since 2018, Professor Chen has been identified as *Highly Cited Researchers* in Cross Field. In 2021, Prof. Chen has been admitted as a *Fellow of The Royal Society of Chemistry* (FRSC).

Jun-Seok Bae

Carbon composites in a honeycomb monolithic structure for CO₂ capture

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Since 2006, CSIRO has developed adsorption-based CO₂ capture technologies, including solid adsorbent material development, process configuration, prototype unit fabrication and site demonstration. For any solid adsorbents, along with high CO₂ capture capacity and high selectivity, they need to be in a certain structural form to reduce operation costs in a process level, minimising a flow resistance (i.e., pressure drop) through a fixed bed, particularly in dealing with high volumetric flow applications that contain moisture and dusts. In this regard, CSIRO has focused on carbon composite development in a honeycomb monolithic structure that possesses continuously open multi-channels along the flow direction and allows a large geometric contact surface area, a low pressure drop, a high dust tolerance and very high resistance to NO_x and SO_x. Various carbon materials have been used to develop carbon composite monoliths, including carbon fibres, carbon nanotubes, biomass and brown coal. The honeycomb structure was made by vacuum moulding and recently extrusion. This presentation will first cover an overview of the journey of CSIRO's R&D on carbon composite adsorbent-based CO₂ capture technology. Then the key results of lab-and large-scale studies, and site trials at a power station will be briefly presented. Lastly, the structural and adsorption characteristics of our carbon composites will be discussed in detail.

Biography



Dr. Jun-Seok Bae is currently a senior research scientist in CSIRO Mineral Resources. He is working with the Environment and Sustainability Research Team in the Sustainable Mining Technologies Research Program. Dr Bae has a PhD in chemical engineering from the University of Queensland (UQ) and specialises in gas separation and purification with solid materials with over 20 years research experiences. Through working at UQ and CSIRO, he has built up extensive research experiences in material and process development, characterisation of materials, enhanced methane recovery from coal seams, flue gas and CO₂ geo-sequestration, ventilation air methane enrichment and biogas cleaning.

Kaige Sun

Capacitive deionization: From ion separation to CO₂ capture

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The whole world is striving to achieve the carbon neutral goal, reducing greenhouse gas emissions, especially carbon dioxide (CO₂) emissions. Electrochemical CO₂ capture technologies are gaining more and more attentions due to their flexibility, energy efficiency and low cost.¹⁻³ Among these technologies, capacitive deionization (CDI) recently showed great possibilities for CO₂ capture and separation, offering low energy consumption and improved capture effectiveness.⁴ CDI is based on electric charge compensation by charged species, which has exhibited promising and exponential growth in the last two decades.⁵ Although CDI has been extensively explored in water desalination/purification and has been used for selective separation of target ions in multicomponent solutions, it suffers lots of challenges towards CO₂ gas capture and separation, such as low electrode capacity, limited understanding of influencing factors, and device design. We will firstly highlight the excellent performance of CDI as water-based technology for water desalination and targeted ion separation, and then transfer to CO₂ gas separation, in which we will show its great possibilities for CO₂ capture and focus on understanding and optimizing CO₂ capture performance.

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Biography



Kaige Sun is currently a PhD student under the supervision of Prof. Xiwang Zhang and Dr. Mike Tebyetekerwa at UQ Dow Centre for Sustainable Engineering Innovation, School of Chemical Engineering, The University of Queensland in Australia, Brisbane. Kaige completed both his bachelor's and master's degree at the Wuhan University of Technology, China. Kaige's current PhD project focuses on electrochemical separation and selectivity, aiming to develop advanced functional materials and devices for efficient electrochemical CO₂ capture and ion separation.

Kristina Konstas

Direct Air Capture with Advanced Porous Materials

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Direct air capture (DAC) is the removal of carbon dioxide (CO₂) directly from the atmosphere. DAC is a critical technology required to meet global net zero targets by 2050. To address this challenge, CSIRO has developed new materials that can selectively capture CO₂. The technology is called, Airthena™, that takes advantage of tiny sponges applied as thin films, requiring only air and electricity to operate. The proprietary thin film composites are applied to electrically-resistive thermal heaters for rapid adsorption and desorption. The first Airthena™ demonstrator captures two tonnes of CO₂ from the atmosphere a year and is suitable for small-scale applications, such as beverage carbonation and industrial cleaning. Our second Airthena™ demonstrator is in development, it is designed to address large-scale applications such as permanent CO₂ removal using underground sequestration. CSIRO has recently launched a Permanent Carbon Locking (CarbonLock) - Future Science Platform. The CarbonLock platform focuses on novel Carbon Dioxide Removal that is scalable, fast-acting, permanent and responsible. An overview of the platform and its activities will be presented.



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Biography Dr Aaron William Thornton is a Principal Research Scientist at CSIRO and Senior Lecturer at Southern Cross University. Specialising in Mathematics, Aaron develops novel and innovative solutions across many topics, including chemistry, materials, engineering, and biology. Bridging the gap between fundamental science, research and industry, Aaron has led several commercial projects and the launch of new products. He has a certificate of entrepreneurship from the Sloan Management School MIT and experience with Venture Capital investors in Energy transition, Healthcare and Digital. Aaron has published in *Nature*, *Science* and other impact journals. He has served as the President of the Membrane Society of Australasia and currently serves on the Editorial Advisory Board for the *American Chemical Society*, *Industrial & Engineering Chemistry Research*.

Lei Ge

Microtubular membrane electrodes for CO₂ electrochemical conversion

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Electrode design is a crucial feature in electrochemical systems. Porous electrodes are required to maximize the reaction sites and participate in reactants delivery, such as gas-diffusion electrodes (GDEs) for gas-phase electrolysis like electrochemical CO₂ reduction reaction (CO₂RR). Planar shape porous electrodes are the conventional configuration with engineering limitations, while microtubular (or hollow fiber) shape electrodes can offer great potential due to several advantages such as a higher active surface area to the volume ratio, small electrolyser footprint, ease of processability etc.

This work covers our recent design and fabrication of Hollow fibre GDEs (HFGDEs) to improve the product selectivity, performance stability, surface wettability, and boost the current density. Firstly we tuned the selectivity of CO₂RR on Cu via controlled electrodeposition of a formate-selective Sn electrocatalyst, revealing the potential of tuning Sn valence state to shift the product selectivity of Cu HFGDE towards formate. To improve the performance stability of Sn-decorated HFGDEs, we develop a strategy to selectively form a distinguished bronze phase via a two-step electrodeposition-annealing process. Since alloys have better chemical and physical stability, bronze HFGDEs could provide a better microenvironment for catalyst-electrolyte contact and therefore a higher current density. To maximise the surface catalytic active sites, we also design the synthesis strategy to build 2D bismuth nanosheets with the abundant surface area on Cu HFGDEs via a controlled pulse electrodeposition technique. 2D Bi nanosheets show 6 times higher catalyst mass activity as compared with bulky shape Bi obtained via usual electrodeposition. On the other hand, to regulate the GDE wettability and improve the efficiency of CO₂RR, we present a wettability regulation strategy that modulates the triple-phase reaction zone in the catalyst layer of GDEs. Some of our ongoing work is focusing on the pore regulation of catalyst layer and gas distribution in GDE.

Biography

I am a current ARC Future Fellow and Associate Professor in the School of Engineering and Centre for Future Materials (CFM) at the University of Southern Queensland (UniSQ). I am currently leading a research team "Gas processing technology and Materials" within CFM, including one Postdoctoral fellow and four PhD students. My research has been focused on material development for gas processing by membrane/adsorption, catalysis and engineering design for addressing the challenges in Australian unconventional gas extraction.

Leo Lai

Structural Evolution of MOF-derived Carbon Catalysts Synthesized by Ultrafast Joule Heating

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Metal organic frameworks (MOFs) have well-defined porous structures and metal-heteroatom coordination, such as metal-nitrogen (M-N) bonds. Pristine MOFs have poor electroconductivities, resulting in low electrocatalytic activities. After high-temperature pyrolysis in an inert environment, MOF-derived carbon materials often demonstrate excellent electrocatalytic activities for various important electrochemical reactions, such as CO₂RR, ORR, OER, and NRR. High-temperature pyrolysis unavoidably involves the removal of O and N species from MOFs and the agglomeration metal species, which strongly influence the activity and stability of resulting electrocatalysts. Standard pyrolysis methods take minutes to hours. Recently, ultrafast heating via Joule heating has been introduced as a new technique to obtain MOF-derived carbon materials with a heating rate of over 10⁵ K/min. The short heating time in seconds may significantly change MOF-derived carbon electrocatalysts.^{1,2} Here, we conduct a systematic study on MOF-derived carbon catalysts synthesized by ultrafast Joule heating compared to those obtained by standard pyrolysis methods. We show that ultrafast Joule heating brings unique structural evolutions, which are strongly correlated with the resulting carbon catalysts' activity and stability in ORR. These findings open a new technique to tailor the properties of MOF-derived carbon electrocatalysts, which can potentially improve their performance for various essential electrochemical reactions.

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Biography



Leo Lai is a Ph.D. candidate supervised by Prof. Yuan Chen and Dr. Li Wei at the University of Sydney. His research focuses on the use of ultrafast heating techniques for the design of carbon based catalysts for key electrochemical reactions such as oxygen reduction reactions.

Lian Zhang

High-Temperature Reactions of CO₂ and Steam with Calcium Chloride

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The fundamental question of whether CO₂ can react with steam at high temperatures in the absence of electrolysis or high pressures is critical in assessing the stability of CO₂ and its capture by Ca-based sorbents such as chloride (i.e., CaCl₂) at high temperature. These two gases are commonly co-present as industrial wastes. Herein, a simple experiment by flowing CO₂ and steam through a CaCl₂ matrix at 500–1000 °C and atmospheric pressure was designed. Comprehensive characterizations and density functional theory calculations were conducted. Meanwhile, this study aims to recover HCl from CaCl₂ via a low-emission oxy-pyrohydrolysis process. As confirmed, CO₂ and steam interact strongly on the CaCl₂ surface, leading to an explicit formation of CaCO₃/CaO and a nearly complete release of HCl. This is mainly contributed to a halved energy required for the splitting of H₂O, resulting from the formation of a bicarbonate-like structure to replace Cl⁻ out of CaCl₂, an otherwise industrial waste, whilst an important dopant for carbon capture, utilization and storage, and medium for electrochemical synthesis. In addition, a micro-fluidised bed reactor was used to assess the kinetic underpinning the reaction of CO₂ and steam with CaCl₂.

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Biography



Professor Lian Zhang is a full-time Professor in the Department of Chemical & Biological Engineering, Monash University. He is the Director of ARC Research Hub for Value-Added Processing of Carbon Waste (ARC-VAP), and Group Leader for Clean Solid Fuel Laboratory (CSFL) focusing on the development of low-emission and high-efficiency combustion and gasification technologies, and flash pyrolysis for the synthesis of bio-fuels and green/turquoise hydrogen from biomass and industrial wastes. Professor Zhang received a PhD degree of Applied Chemistry from Nagoya University Japan in 2004. He is always interested in the development of new technologies, as well as the understanding of the science underpinning the technologies under development.

Liang Sun

High Entropy Alloy Enables Efficient CO₂ Redox Reactions

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The performance and cyclability of lithium-CO₂ (Li-CO₂) batteries have been limited by high overpotentials and low discharge capacities. Here, we report the development of a high entropy alloy (HEA) as a novel cathode material for Li-CO₂ batteries. The HEA is composed of five metals with high mixing enthalpy and configurational entropy, leading to enhanced electrochemical activity and stability. Our results show that the HEA cathode significantly reduces the overpotential of Li-CO₂ battery and improves its long-term cyclability over 2000 hours. The excellent electrochemical performance of the HEA cathode is attributed to its high electrochemical surface area, porous structure, and enhanced catalytic activity towards CO₂ redox reaction. This work provides a promising strategy for developing high-performance cathode materials for Li-CO₂ batteries, and opens up new avenues for the design of HEA-based materials for energy storage applications.

Biography



Liang Sun is currently a PhD student in the University of Adelaide, Adelaide, Australia. His research focuses on the design and fabrication of novel materials in new-generation energy storage and conversion, such as Li-CO₂ batteries.

Liu Ye

Towards Net-zero Emissions in Urban Water Industry

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The water industry is a major contributor to global greenhouse house gas (GHG) emissions and is now ranked as the 7th largest contributor to the global anthropogenic GHG budget. The water industry is setting targets to achieve net-zero emissions by at least 2050 and some as early as 2025. Water industry's push for net-zero operation is an essential step towards creating a more sustainable and environmentally friendly future. By adopting more sustainable practices and reducing its carbon footprint, the industry can help protect our planet's environment while still meeting the growing demand for safe and clean water. This talk will focus on sharing state-of-the-art knowledge, practical experience from the GHG team at the University of Queensland (UQ), together with the Australian water utilities, in managing fugitive greenhouse gas emissions from urban water industry in the past decade. It will also discuss challenges and opportunities lie in our future in achieving net-zero emissions in water sector in the coming years.

Biography



Dr. Liu Ye is an Associate Professor at The University of Queensland (UQ) in the School of Chemical Engineering. Dr Ye's research is focused on sustainable environmental engineering and is dedicated to finding innovative and practical solutions to tackle challenges in achieving net zero emissions, climate resilience, and sustainability. She is the Greenhouse Gas (GHG) research program leader at UQ urban water engineering and has an established national and international leadership in this field. Her research have made significant contributions in the quantification, modelling, and mitigation of greenhouse gas emissions in urban water systems and the research outputs are used by Australian water utilities in full-scale treatment plants to reduce the fugitive GHG emissions.

Matthew Kratzer

Species-dependant diffusion in flue gas separation through carbon nanotube arrays

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The current worldwide demand for the increased utilisation of renewable energy requires new energy transport and storage technologies. The storage and separation of waste gases, such as flue gases, is becoming increasingly important as a decarbonization method. Nanoporous materials are receiving increasing interest as membranes for gas separation, due to the associated low interfacial resistance and high selectivity.

In this presentation I will discuss some models of gas transport through ideally-ordered nanomaterials, such as vertically aligned carbon nanotube arrays. The primary outcomes of this work are the development of a surface scattering kernel for free-molecular gas transport through such nanomaterials, along with a Fokker-Planck model which accounts for the non-Fickian behaviour of gas flowing through the entrance region of carbon nanotubes.

The results of this analysis predict that simple gas molecules, such as H₂ and CO₂ experience higher friction in such systems in comparison with larger hydrocarbons such as CH₄. The results are proposed as a potential explanation of the reduced gas transport of hydrogen gas in nanoporous systems.

Biography



Matthew is an early career researcher currently focused on the modelling of hydrogen storage and transport. Matthew is currently completing his PhD on nanoscale gas transport, focusing on particle-surface interactions.

Mengran Li

Designing inherently stable PGM-free CO₂ electrolysis

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CO₂ electrolysis is a promising electrochemical route to convert waste CO₂ into useful products such as CO, C₂H₄, or ethanol. Research efforts over the past decades have greatly improved its reaction rate close to the industrially applicable rate through catalyst development, electrode innovation, and cell configuration re-design. The state-of-the-art electrolysis cells are built based on monopolar ion-exchange membranes and are designed to achieve a pH-neutral or alkaline local reaction environment at the cathode, which is the centre for CO₂ reduction to take place. However, these cell designs are inherently unstable, causing either significant salt precipitation that blocks CO₂ at the cathode or dissolution of the PGM-free catalysts that destabilise the anode. This talk will report our recent work to address this critical stability issue by applying bipolar membranes to enable stable PGM-free electrolysis cells for CO₂ electrolysis. I will first explain the important role of electrochemical engineering design and ion-exchange membrane in predetermining the local reaction microenvironment and then discuss the new challenges and opportunities in catalyst design and membrane development for inherently stable electrolysis.

Biography



Dr Mengran Li is a lecturer and ARC DECRA in the Department of Chemical Engineering. After graduating with his PhD at UQ in 2016, he worked as a postdoc research fellow at UQ, working on the development of CO₂ electrolysis technology for the iron-steel company for more than three years. In 2021 he joined the Delft University of Technology, the Netherlands, as another postdoc continuing his research on CO₂ electrolysis supported by the EU Horizon Project. He then joined the Chemical Engineering Department at the University of Melbourne and was awarded ARC DECRA in 2023.

Michael D. Guiver

MOFs and microporous polymer frameworks for gas separation membranes

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Gas separations, particularly CO₂¹ and olefin/paraffin separations, are of interest for environmental protection, process efficiencies, and energy reduction. As membrane materials, the current utilization of MOFs and COFs needs improvements in practicality and scale up. We focused on CO₂ and olefin/paraffin separations using design principles such as gas-selective channel architecture and supported ultrathin gas selective layers. MOFs and microporous polymer frameworks (MPF)² employed in mixed matrix membranes (MMM) are constructed with 'direct channel' methodology³, in which filler particles protrude through the polymer matrix; gas transport is governed mainly by the filler, improving both gas permeance and selectivity. MPF fillers with amine-rich nanochannels interact specifically with CO₂⁴. Apart from MMMs, the practical use of MOFs is achieved by growth of larger-area ultrathin gas selective layers grown onto conventional flexible polymeric ultrafiltration membrane supports^{5,6}, which exhibit very high gas permeances. Other MOF glass-foam membranes were explored for high permeance methane-selective CH₄/N₂ separations⁷.

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Biography



Michael D. Guiver obtained his PhD in Polymer Chemistry from Carleton University in 1988. He served as Editor for the *Journal of Membrane Science* from 2009–2020 (12 years). He is now the inaugural Field Chief Editor for *Frontiers in Membrane Science and Technology*. He is a Fellow of the Royal Society of Chemistry, an ACS Poly Fellow, and was awarded Fellow of the North American Membrane Society for technical achievements and service to the society. From 1987–2014, he was a scientist at the National Research Council Canada. In 2009–2013, he was a visiting professor at Hanyang University, Korea. In September 2014, he took a full-time position at the State Key Laboratory of Engines, Tianjin University, China. His research focus is membrane materials for fuel cell and gas separations.

Mohamed Nazmi Idros

Catalyst layer ink formulation matters for CO₂ electrolysis

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This study delves into the impact of solvent-ionomer interactions within the catalyst ink on catalyst layer (CL) properties, including its structure, wettability, and performance in CO₂ electrolysis. Our results reveal a distinct behaviour: acetone demonstrates a stronger solvation effect on the hydrophobic perfluorinated sulfonic acid, Aquivion® backbones than methanol. Consequently, when we cast a mixture of Aquivion® and acetone on a flat surface, the resulting ionomer film is more continuous and hydrophobic than its methanol counterpart. This interaction also translates to a more uniform and flood-resistant gas diffusion electrode when we produce the copper catalyst layer with acetone (acetone-CL) compared to methanol (methanol-CL). As a result, the acetone-CL displays a higher selectivity for CO₂ electrolysis to C₂₊ products at high current density, outperforming the methanol-CL by up to 25% at 500 mA cm⁻². This improved selectivity can be attributed to the acetone-CL's superior resistance to electrolyte flooding, with zero seepage observed even at the highest tested current densities. Furthermore, we investigate the role of polytetrafluoroethylene (PTFE) in shaping solvent-ionomer interactions within the CL formulation. Our results suggest that introducing PTFE into the catalyst layer (CL) not only improves gas transport but also disturbs the interactions between the solvent and ionomer, leading to changes in the microenvironments within the CL. These insights shed new light on a previously overlooked aspect and open promising avenues for tailoring CLs to achieve enhanced performance in CO₂ electrolysis.

Biography



Mohamed Nazmi Idros is a PhD student in the School of Chemical Engineering at the University of Queensland, Australia, under the supervision of Associate Professor Tom Rufford, Dr Mengran Li and Dr Tim Duignan. Nazmi received his Bachelor of Engineering in chemical engineering from the University of Queensland in 2019. His current research interest is understanding ionomer characteristics in the formulation and catalyst layer for CO₂ electrolysis.

Muxina Konarova

Enabling Hydrogen Storage and Transport: Unleashing Cost-Effective Potential through Liquid Organic Hydrogen Carriers

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Liquid Organic Hydrogen Carriers (LOHCs) stand out as one of the most economical and safe alternatives for hydrogen transportation. This technology, relevant at large scale, relies on a hydrogen carrier's cyclic hydrogenation ($\text{LOHC} \rightarrow \text{LOHC}^+$) and dehydrogenation ($\text{LOHC}^+ \rightarrow \text{LOHC}$). However, nowadays, the hydrogenation of the LOHC still requires a source of H_2 , with high purity, i.e., >99%, and pressure, e.g., $P \geq 30$ bar. Thus, simply transporting H_2 via LOHC will not turn the economic scales of H_2 widespread usage. The main reasons for using pure H_2 for hydrogenation are related to metal-based catalyst stability, as is the high H_2 pressure [1]. Indeed, typical impurities in raw H_2 -rich streams from biomass include CO and H_2S (known poisons for most metal catalysts), H_2O (promotes metal sintering), CO_2 (can be transformed via H_2 over metal-based catalysts into CO , H_2O , and CH_4 , decreasing H_2 recovery and causing catalyst deactivation), CH_4 , and other inert gases, like N_2 . Therefore, the development of stable catalysts in the presence of raw H_2 impurities and under milder conditions would open the door for direct use of LOHC hydrogenation. Hydrogenation of organic molecules require metal particles to be present in the catalyst, these are now exclusively dedicated to activating H_2 molecules which mainly focused on noble metals such as Pt on alumina, Pd on sodalite [2]. These noble metals were encapsulated in small pore zeolites to prevent the deactivation of the metallic phase by poisoning, sintering, and coke deposition. Nowadays, no catalyst exists to use LOHC hydrogenation for effective raw H_2 purification. While hydrogen splitting over Pt/zeolites can be a viable solution, these noble metals are expensive and very sensitive to impurities. In addition, the most Pt/zeolite -based catalysts for LOHC reaction suffers from coking and thus require frequent regeneration by burning the coke which will make significant amount of CO_2 and metal sintering/loss of surface area. In this talk, types of catalysts suitable for liquid organic hydrogen carriers will be presented, with a focus on hydrogenation of N-ethylcarbazole using catalysts.

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Biography



Dr Muxina Konarova is a Senior Lecturer at The University of Queensland (UQ) in the School of Chemical Engineering. She gained her PhD in Chemical Engineering at Tokyo Institute of Technology, Japan. Since 2016, Dr Konarova has attracted >\$3M in competitive research funding as a Chief Investigator, including ARC Linkage, ARC Discovery and ARENA grants. Dr Konarova has received a Monash Engineering Women's Leadership Award (2016) and represented Australian early/mid-career researchers at the VI World Materials Summit (2017) in Strasbourg, France.

Neil Robinson

Low-field time domain NMR of porous systems

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Functional porous materials underpin a vast range of critical chemical processes, ranging from fuel storage, to the production of materials and chemicals from renewable resources. The underlying chemical and physical processes associated with such applications are a direct result of the interactions of these porous structures with fluids (gases, and/or liquids) via their encapsulation, surface adhesion, and/or chemical reaction. Despite their ubiquity and high industrial and socioeconomic importance, however, notable knowledge gaps remain regarding the properties of fluids confined within such materials. Indeed, the characterisation of chemical reaction and interaction phenomena occurring within the void spaces of optically opaque porous structures remains one of the most significant challenges in physical science and engineering, requiring measurement approaches with the ability to reliably discriminate between molecules interacting with the interface(s) of interest, and the surrounding solid and fluid components. This talk will provide an introductory overview of to the application of low magnetic field nuclear magnetic resonance (NMR) relaxation measurements to such problems, which provide a versatile, non-invasive and chemically selective approach with which to characterise fluid interactions within porous solids, and which may be implemented under operando pressure and temperature conditions of direct relevance to industrial chemical processes. Such measurements have been employed by the rock physics and hydrocarbon recovery community for over five decades, but their application to well-defined functional porous materials has until now been extremely limited. Correspondingly, this talk will describe recent applications of nuclear spin relaxation to systems of relevance to catalysis [1-3] and gas process engineering [4], highlighting potential avenues for the application of such measurements to systems of relevance to CO₂ transformations.

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Biography



Dr Neil Robinson is a Research Fellow within the Fluid Science and Resources Research Group at the University of Western Australia (UWA). He received his PhD in Chemical Engineering from the University of Cambridge, following which he relocated to UWA to work with Prof Mike Johns on magnetic resonance-based methods to characterise functional porous materials of importance to the energy-environment nexus; in 2022 he was awarded a prestigious Forrest Research Foundation Fellowship to continue this research direction. Neil received the 2022 Australian National Measurement Institute (NMI) Prize, was a finalist in both the 2021 and 2022 IChemE Global Awards, and represented Australia at the 71st Lindau Nobel Laureate Meeting.

Ngoc N. Nguyen

Unconventional CO₂ Capture Based on Gas Hydrates

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CO₂ capture (or carbon capture) is important for decarbonising the world. However, adapting the existing CO₂ capture technologies in chemical industry to environmental applications leads to unfeasible costs. This bottle neck has driven intensive quests for alternative methods for cost-effective carbon capture. Gas hydrates present a novel pathway for efficient carbon capture by allowing a large amount of CO₂ to be encapsulated in regular cavities of hydrogen-bonded water network to create a CO₂-carrying solid material (called gas hydrate) with a mass fraction of CO₂ being up to 30 %. The resulting gas hydrate is then dissociated to recover the CO₂ for utilisation. The selective capture (i.e. separation) of CO₂ from a gas mixture is enabled by its higher affinity to form gas hydrate compared to other gases. Such a hydrate-based carbon capture has intrinsic competitive edges, for example, it is a water-based process and being environmentally friendly. In this talk, I will present the key concepts, the latest advances, the prospect, challenges and future directions of research toward enabling this unconventional carbon capture method in the context of a low-carbon economy.

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Biography



Ngoc N. Nguyen obtained a PhD in Chemical Engineering from The University of Queensland (UQ) in 2018. Currently, he is a research fellow and upcoming ARC DECRA Fellows (2024-2027) at UQ. He was an Alexander von Humboldt Fellowship and worked for Max Planck Institute for Polymer Research in Germany for three years (2019 – 2021). He used to work as a visiting scholar to Pacific Northwest National Laboratory in USA and a lecturer at Hanoi University of Science and Technology in Vietnam. His research focuses on surface science and multiphase physics for applications in the field of green energy, resources, minerals processing and carbon capture in the broader breadth of low-carbon technologies and circular economy.



Anh V. Nguyen is a full professor in the School of Chemical Engineering, UQ. He was an ARC (Australian Research Council) QEII (Queen Elizabeth II) Fellow and then an associate professor at the University of Newcastle, Australia, and has held many adjuncts and visiting positions overseas, including those at the University of Utah (USA), Central South University (China), and Kyushu University (Japan). He obtained his Ph.D. in (the former) Czechoslovakia and then worked under an Alexander von Humboldt Research Fellowship at the Max Plank Institute for Colloids and Interfaces, Germany. His research is concerned with applied colloid and surface chemistry in chemical engineering. He published one book on the colloidal science of flotation and more 340 peer-reviewed journal papers and book chapters

Penghui Yan

Influence of supports and metal particle size on CO₂ methanation

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Increase in the concentration of CO₂ on Earth's atmosphere results in detrimental effects, posing a significant threat to various life forms. Consequently, considerable efforts are being dedicated to addressing CO₂ emissions and their repercussions. One practical approach for CO₂ mitigation involves the hydrogenation of CO₂ to produce methane, also known as synthetic natural gas (SNG) [1]. Methane is a promising hydrogen carrier due to its well-established liquefaction process in addition to its safe transportability. Many researchers have concentrated their efforts on CO₂ methanation with a specific focus on nickel catalysts supported by diverse materials [2]. These studies aimed to evaluate their activity, stability, and potential industrial applications. Zeolites have proven effective as carbon dioxide adsorbents, particularly at temperatures ranging from 250 to 300 °C.

In this study, the hydrogenation of CO₂ over Ni-based catalysts with varied supports was meticulously investigated in a continuous flow reactor. The outcomes of this investigation revealed that the choice of support significantly influences the production distribution, primarily attributed to the difference in metal particle sizes. As shown in Figure 1, catalysts with small pore diameters (<1 nm) such as 5Ni-4A, 5Ni-5A, and 5Ni-13X exhibit larger metal particle sizes, thereby enhancing the hydrogenation activity and resulting in higher methane yields. In contrast, catalysts with larger pore diameters (>1 nm) and greater surface areas, like 5Ni-ZSM-5 and 5Ni-BETA, exhibit lower nickel particle sizes. Consequently, these catalysts show reduced hydrogenation activity, a lower selectivity towards methane selectivity, but an increased selectivity towards CO.

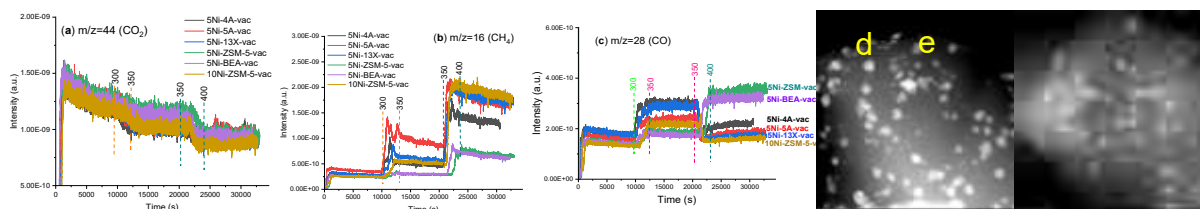


Figure 1. In situ mass spectrometer analysis of the (a) CO₂ (m/z=44), (b) CH₄ (m/z=16), and (c) CO (m/z=28), HAADF-STEM images of (d) 5Ni-ZSM-5 and (e) 5Ni-13X.

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Biography



I obtained my MSc from University of Chinese Academy of Sciences in 2013 and PhD degree in Chemical Engineering from the University of Newcastle in 2020. Currently, I am a research fellow at the University of Queensland. In the past 10 years, I have been engaged in the field of heterogeneous catalysis, with a specific focus on renewable energy. My research interests include CO₂ hydrogenation, biomass catalytic pyrolysis, biofuel upgrading.

Porun Liu

Single Atom Catalyst for Efficient Hydrogen Evolution and Oxygen Reduction Reactions

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Fabrication of highly dispersed monoatomic active sites on high surface area of two dimensional (2D) materials has emerged as an effective approach toward high performance catalysis. The catalytic activity of the single atom catalysts depends strongly on the metal centres and their adjacent chemical environment. Herein, we demonstrate the fabrication strategies to effectively anchor active transition metal (TM = Mn, Fe, Co, Ni, Cu, Ru) single atoms (SAs) on 2D matrix (graphitic carbon, MXene) with uniformly dispersed active sites. More importantly, by regulating the metal centres and the substrates, the adsorption of the reaction intermediate on the single atom catalysts has been optimized towards hydrogen evolution reaction (HER), oxygen reduction reaction (ORR). The improved electrocatalytic activities of the SACs afford high performance of hydrogen production in alkaline solution and zinc air batteries.

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Biography



Porun Liu received his Ph.D. in chemical science in 2011 from Griffith University. He subsequently worked as a Research Fellow in the Centre for Catalysis and Clean Energy. He was awarded a Griffith University Postdoctoral Research Fellowship in 2015 and an Australian Research Council Discovery Early Career Researcher Award in 2017. He is currently the Deputy Director of Centre for Catalysis and Clean Energy and an Associate Professor in the School of Environment and Science, focusing on synthesis, in situ characterizations, and electrocatalytic applications of nanostructured catalysts in energy conversion and storage devices.

Qi Gao

Integration of CO₂ Capture and Electrochemical Conversion

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Carbon dioxide capture (CO₂) from a point source or air is an essential step to decarbonise the economy. The captured CO₂ can then be potentially used as feedstock to produce valuable chemicals through electrochemical conversion combined with renewable energies. However, this sequential CO₂ capture and electrochemical conversion is usually formidably energy costly. The solvent regeneration is usually the most energy-intensive step in the CO₂ capture process, contributing up to 90% of the overall energy for the most commercially mature amine scrubbing process. Additionally, the pure CO₂ gas feed into the CO₂ electrolyser can form (bi)carbonate at the cathode², which can cause instability and low efficiency of the electrolyser³.

Recently, the integrated CO₂ capture and conversion process is being considered as a promising process to reduce overall energy costs. This integrated process has the potential to allow the energy-intensive regeneration step in CO₂ capture to be replaced by the electrolyser, and (bi)carbonation formation in the electrolysis to be avoided by eliminating the presence of pure CO₂ gas feed. This poster will provide an in-depth review of the integration of CO₂ capture and electrochemical conversion. I will first compare the associated mechanisms and energy benefits of different integrated electrolysis processes. Then I will summarise recent advances to improve product selectivity and current densities of the integrated electrolysis through innovating solvents, catalysts, temperatures, and pressure. This poster will conclude with challenges in regenerating the capture solvents from electrolysis and opportunities in selecting membrane and cell configurations.

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Biography



Qi Gao completed her BEng in Applied Chemistry from Dalian University of Technology and her MEng in Chemical Engineering from the University of Melbourne. Her current research focuses on developing an integrated CO₂ capture and electrolysis system.

Qian Sun

Enhanced C₂₊ Production from CO Electroreduction by Using Molecular Doping

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Electrochemical reduction of CO₂ is promising to convert CO₂ into valuable chemicals. Most studies are devoted to CO₂RR in highly alkaline electrolytes to suppress hydrogen evolution reactions and improve reaction kinetics. However, this technology is challenged by carbonate formation by CO₂ interaction with OH⁻, which induce significant reactant loss and large energy penalty for CO₂ recovery. This can be addressed by CO electrochemical reduction reaction (CORR), which avoid carbonate formation, afford stable operation under alkaline conditions, and benefit C₂₊ production. Nonetheless, the activity and selectivity for CO-to-multi-carbon products conversion remain low due to the lack of efficient catalysts. Atomic Cu-Au alloy with isolated Au atoms on Cu support is effective in catalysing CORR ¹, attributed to the unique geometric and electronic structure of atomic Cu-Au interfaces which afford improved acetate activity and selectivity. To boost the multi carbons production, molecular doping was deployed to modify the surface of Cu-based catalysts ². Therefore, functionalizing the surface of the atomically dispersed Cu-Au alloy with aromatic heterocycle can further improve the production of C₂₊ species from CORR.

Herein, we employed thiadiazole derivate (N₂SN) to modify the atomic Cu-Au alloy (CuAu_{1%}), obtaining CuAu_{1%}+N₂SN for CO electroreduction into C₂₊/acetate. Using which, high Faradaic efficiency (78.8%) and maximum partial current density (422.8 mA cm⁻²) for C₂₊, as well as that (57.4%, 307.9 mA cm⁻²) for acetate were achieved, surpassing the sample without molecular doping and most of the reported Cu-based catalysts. In situ Raman revealed that the N₂SN introduction contributes to higher *CO coverage than the unmodified sample, promoting the further dimerization of *CO for C₂₊ species. Besides, stronger C-C-O intermediate peak was detected for CuAu_{1%}+N₂SN, suggesting higher acetate production. The N₂SN of electron deficient property could alternate the oxidation state of the surface Cu atoms, thereby promoting acetate formation.

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Biography



Qian Sun is currently a PhD student in Prof Chuan Zhao's group in UNSW, her research focuses on electroreduction of CO₂ and CO using single atom catalysts. Up to date, she has published several papers in Chemical Communications, ACS catalysis, Applied Catalysis B: Environmental, Chinese Journal of Catalysis, and Encyclopedia of Ionic Liquids.

Qin Li

Biomass to Catalytic Quantum Materials: Enriching the Pathways for CO₂ Conversion

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Solar-to-fuel is the ultimate route for reducing our carbon footprint and mitigating climate change. In this process, biomass can play an important role by an appropriate utilization strategy. The global annual generation of agricultural and forestry biomass waste is on the order of 140 Gt, and Australia produces over 130 Mt per year according to the Australian Bureau of Statistics. Currently, in Australia more than 90% of the agriculture and forestry biomass waste is burned or wasted, causing major negative climate and environmental impact. With the increasing investment into H₂ economy infrastructure, biomass-derived fuels can be designed to be compatible and supportive to the rising H₂ economy for achieving zero-carbon emission. For example, biomass-derived fuels and chemicals can be utilised as liquid hydrogen carriers through catalysis-enabled reversible dehydrogenation and hydrogenation. This talk will focus on photocatalysis-enabled on-demand hydrogen release from methanol. In this sustainable technology development, the design, synthesis, and life-cycle analysis of the photocatalysts are of critical importance. While the catalysts should be highly efficient, the catalysts themselves should also comply with green chemistry principles to be genuinely environmental. Carbon quantum dots, nanosized graphitic carbon materials, are one of the excellent candidates to fulfill this role. Two types of carbon dots-based semiconductor materials will be introduced, and two types of photocatalytic reactions will be illustrated with one being aqueous-based and the 2nd organic solvent-based.

Biography



Dr. Qin Li is a Professor at Queensland Micro- and Nanotechnology Centre, and School of Engineering and Built Environment, Griffith University. She is the co-founding chair of the Green and Sustainable Chemistry & Engineering National Group at Royal Australian Chemical Institute. Her research interests span from nanocarbons, colloids and interfacial engineering, to functional materials, catalysis, and sustainable technologies, addressing wide application fields in water, energy and healthcare.

Qingbing Xia

Probing Electronic-Scale Charge Storage Mechanisms via Electron Paramagnetic Resonance

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Electron paramagnetic resonance (EPR) spectroscopy offers exceptional sensitivity to both the density and the surrounding environment of unpaired electronic spins, rendering it a highly valuable technique for characterising chemical alterations in electrode materials. Different from conventional characterisation methodologies such as X-ray diffraction (XRD), transmission electron microscopy (TEM), and Raman spectroscopy, which typically offer only constrained insights into material structure, EPR has the unique capability to monitor dynamic reactions at the electronic level. This capability enables EPR to furnish a profound comprehension of the structural environments inherent to the materials under investigation. This presentation will disseminate our most recent research findings, which revolve around comprehending the Na ion storage mechanisms in hard carbon materials at the electronic level, employing the EPR technique as a pivotal investigative tool by which we are able to delineate and distinguish the processes of Na ion intercalation, adsorption, and clustering within hard carbon materials. Consequently, our research contributes to a revised understanding of the Na ion storage mechanism in hard carbon. Our findings substantially enrich the understanding of charge storage in electrode materials, offering new insights into the characterisation of electrode materials for energy storage and conversion applications.

Biography



I earned my B.Sc. and M.Sc. degrees in Materials Science and Engineering from Central South University (China) in 2012 and 2015, respectively. In 2019, I completed my Ph.D. at the University of Wollongong (Australia). In July 2020, I started my postdoctoral research at The University of Queensland. My current research interests focus on the development and application of in situ techniques for studying charge storage mechanisms in electrodes for electrochemical energy storage applications.

Quang Kim Loi

Reaction dynamics and molecular transport of CO₂ hydrogenation on N-doped graphene using ReaxFF simulations

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There is considerable interest in designing next-generation catalysts for the conversion of CO₂ into high-level products. Recently, N-doped quantum-dot graphene has demonstrated some unusual selectivity to the formation of CO and CH₄ rather than methanol from hydrogenation of CO₂ [1]. In this study, we performed ReaxFF molecular dynamics (MD) simulations to investigate the reaction dynamics and the transport properties of reactant and products on the catalyst's surface. The use of a ReaxFF force field allows for the modelling of reaction and calculation of transport properties within a meaningful timescale and at reasonable computational costs as opposed to the more intensive DFT and *ab initio* MD simulations. Both transport and self-diffusion coefficients are calculated as a function of temperature for different operating conditions. In addition, local properties such as species distribution and local mobility are explored to investigate possible improvements.

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Biography



Dr Quang Kim Loi obtained his PhD degree from the School of Chemical Engineering at the University of Queensland in 2021. He is currently a postdoctoral research fellow at the Bernhardt group at the Australian Institute of Bioengineering and Nanotechnology. His research focused on using molecular simulations to understand the molecular behaviour and transport properties at the interfaces and in nanoporous materials.

Rana Arslan Afzal

Investigating the impact of various treatments on the lignocellulosic biomass and its derived carbon features

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Carbon is flexible and widely utilised in many applications. Thus, worldwide demand for new and enhanced carbon materials is rising. Carbon materials have traditionally been made from fossil fuels, but these sources are becoming scarce and increasingly unsustainable. Naturally abundant lignocellulosic biomass is emerging as an attractive alternative carbon precursor. Due to their abundance, cost-competitiveness, and renewable nature, numerous agricultural residues are being investigated as organic biomass sources for a more sustainable future. The uses of carbon materials rely on their structure and qualities. Traditional carbonisation parameter optimisation controls these features. Most of the research to-date has been based on direct carbonisation (pyrolysis) of biomass, and few studies address pyrolysis parameter management to maximise carbon structure and yield. However, a few more recent studies are showing how careful selection of plant tissues with varied biomass treatments can affect the structure and characteristics of carbon. The most significant biomass treatment procedures are delignification (chemical pulping) and fibrillation (mechanical refining), which impact valorised carbon characteristics. No systematic study has established a structure-processing-property-performance connection for biomass-derived carbon that encompasses *both* chemical pulping and mechanical refining. A deeper knowledge of these processes will allow process control and optimisation for high-yield carbon material manufacturing with customised morphologies and attributes for specific applications. Our research hypothesis is that the selection of a combination of (a) sorghum plant tissue selection, (b) lignocellulose content, and (c) biomass fibrillation degree can lead to optimal hard carbon performance in supercapacitors. Thus, using sorghum as a non-wood agricultural residue precursor, this research seeks to fill this knowledge gap and develop more advanced methods to process and “tune” hard carbon materials for energy storage (i.e., as competitive supercapacitor anodes).

Biography



Rana Arslan Afzal's PhD research focuses on valorising carbonaceous energy materials from non-wood biomass sources to develop sustainable precursors for future energy materials. His research interests include Energy materials, Biomass-derived carbon, and Functional nanomaterials.

Ravichandar Babarao

Accelerating the Discovery of Novel Materials for CO₂ Capture: Integrating High Throughput Simulation and Machine Learning

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Porous materials especially, coordination polymers (CP) or metal-organic frameworks (MOFs) have emerged as a special class of hybrid nanoporous materials. The variation of metal oxides and the vast choice of controllable organic linkers allow the pore size, volume and functionality of MOFs to be tailored in a rational manner for designable architectures. MOFs thus provide a wealth of opportunities for engineering new functional materials and are considered as versatile candidates for storage, separation, sensing, catalysis, drug delivery and other important applications. With ever-growing computational resources and advance in mathematical techniques, molecular simulations have become an indispensable tool for materials characterization, screening and design. At a molecular level, simulations can provide microscopic insights from the bottom-up and establish structure-function relationships. This presentation will highlight on how molecular modelling combining with machine learning approach can a powerful tool in complementing experiments and thus aid in designing of new smart porous materials for CO₂ storage and separation.

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Biography



Dr. Ravichandar Babarao, (Senior Lecturer) leads the Molecular Modelling Team, School of Science, RMIT University, Melbourne, Australia. He received his PhD from National University of Singapore in 2010 before joining Oak Ridge National Laboratory (ORNL) as a Postdoctoral Research associate in chemical science division. Then in 2012, he moved to CSIRO as a postdoctoral research fellow and then promoted to Research Scientist in 2014 before moving to RMIT in 2016. In recognition of his outstanding contribution to energy and environmental sustainability, he was awarded the *2015 Prosper.net Scopus Young Scientist Award* in the Energy category among Asia –Pacific region. He was also awarded the the prestigious Alexander von Humboldt Fellowship to spend time in research institutes in Germany for 6-18 months. In addition, he was awarded the *2016 RACI Rennie Memorial Medal* and a *Victoria Fellowship* from the Victorian government for his excellence in research in Chemical and Physical Science. He was awarded the *2019 Peter Schwedtfeger Award* from the Australian Association of von Humboldt Fellows. He was one among the fifteen researchers to be named in the *2020 Class of Influential Researchers* from Industrial Engineering and Chemistry Research. His current area of research is to use state of the art computational techniques for accelerating the discovery of novel robust porous materials, in particular metal–organic frameworks or porous coordination polymers for sustainable energy and environmental applications.

Rijia Lin

Glassy Metal-Organic Frameworks: New Opportunities in Membrane Gas Separation and Devices

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Typically, metal-organic frameworks (MOFs) are hybrid crystalline materials with metal nodes connected by organic ligands. Recently, the melting behaviour of MOFs has attracted increasing research interest. Glassy MOFs are an emerging family of MOFs with the crystal-liquid-glass transformation capability upon heating and the subsequent vitrification during cooling.¹ The thermal rheological behaviour of MOF glass endows unprecedented features that most crystalline MOFs have not exhibited, including high processability, reactivity and dynamic microporous structure evolution.² The access to the liquid phase of glassy MOFs allows for more flexible processing of MOF devices and compositing with other functional materials, overcoming a significant barrier to the practical application of MOFs.

This work will introduce our studies in glassy MOF composite materials for membrane separation and devices, focusing on optimizing the composite interface. We developed a MOF glass mixed matrix membrane by *in situ* melting of ZIF-62(Zn) within the polyimide matrix.³ The *in situ* melting of glassy MOF effectively healed the defects at the MOF-polymer interface, which led to a 57% increase in CO₂/N₂ selectivity for the composite membrane compared to the pure polymeric counterpart. Utilising the reactivity of MOF liquids, a bimetallic MOF glass hybrid was prepared by melting the ZIF-62(Co) together with an adsorbed ferric coordination complex.⁴ The reactive ZIF-62(Co) liquid facilitates the formation of coordinative bonds between Fe and imidazolate ligands. Moreover, by utilising the reactivity of ZIF-62, we introduced a facile mechanochemical technique to produce MOF glass coatings on carbon cloth for fabricating larger area electrodes.⁵

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Biography



Dr Rijia Lin is an Australian Research Council (ARC) Discovery Early Career Research Fellow at the School of Chemical Engineering, The University of Queensland. Dr Lin obtained his B. S. and M. S. degrees from Sun Yat-sen University (China) in 2010 and 2012, respectively, and his PhD from the University of Queensland in 2016. His main research interests include metal-organic frameworks, membrane gas separation, and porous glass materials.

Rosalie K. Hocking

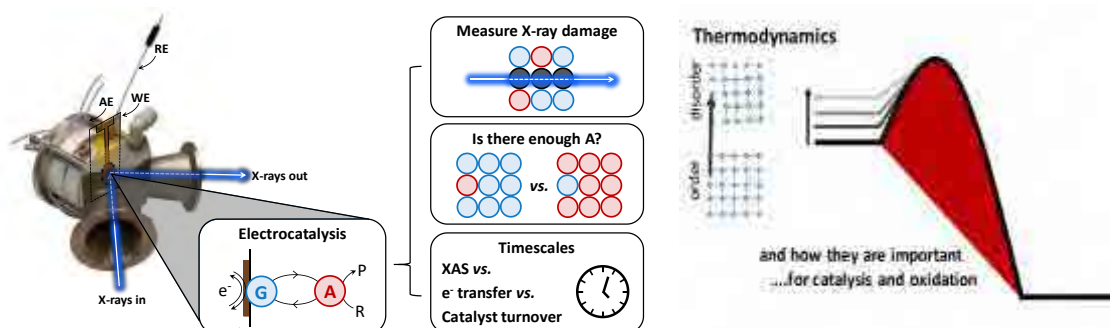
In designing catalysts for clean energy- is the nature of the active site always the right question to ask?

Rosalie K. Hocking¹

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One of the greatest challenges of the 21st century will be securing cheap and renewable sources of energy. One of the most promising approaches to this challenge is to design catalysts from earth-abundant materials capable of implementing key chemical reactions, including splitting water into hydrogen and oxygen ($\text{H}_2\text{O} \rightarrow 2\text{H}^+ + \text{O}_2$); and both the oxidation ($\text{H}_2 \rightarrow 2\text{H}^+$) and reduction ($2\text{H}^+ \rightarrow \text{H}_2$) of hydrogen and the chemical reduction of carbon dioxide among many others. In studying catalysts, we often focus on the “nature of the active site” which for classical heterogeneous catalysts works well- but not all catalysts work by a surface sorption process alone. In some systems, it is increasingly realised that processes of precipitation and reformation may actually be key to catalysis. In this talk we explore the relationship between redox chemistry and catalytic chemistry using a range of catalysts as examples including nickel single atom catalysts, birnessite-like manganese oxides and iron sulfides. We fundamental differences between material and how they transport electrons for electrode to substrate. Using synchrotron based XAS as a tool we explore key redox events between substrates and catalyst and the speed of these processes and how it impacts product selectivity and catalyst stability. We examine how the events after catalysis may be key for understanding the active events of catalysis as well as mechanisms of decomposition.



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Biography

Rosalie Hocking is a chemist whose research is aimed at the development of electrochemical devices to make commodity chemicals (like hydrogen and ammonia) from solar-derived electricity. Her work makes extensive use of the Australian Synchrotron where she uses X-rays to find out how new materials work, and why sometimes they don't! She is also researching the development cheap sensor devices that would provide instantaneous chemical information, important in applications like Asbestos identification on building sites. Rosalie completed her PhD in physical and inorganic chemistry from the University Sydney in 2004. She has since held positions Stanford University/Stanford Synchrotron Radiation Laboratory, CSIRO Land and Water, Monash University and James Cook University before coming to Swinburne University of Technology. She is currently a senior lecturer in chemistry and deputy department chair of Chemistry and Biotechnology.

Ruiqi Chen

Ion Incorporation in ZIF-62 Glasses: Melting Behavior, Interaction Dynamics, and Enhanced Gas Separation Performance

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Metal-organic framework (MOF) glasses, such as ZIF-62, have attracted significant attention due to their unique porous nature that persists even during phase transitions between liquid and solid states. ZIF-62 is renowned for its ultrahigh glass-forming capabilities and a distinct melting-to-decomposition temperature difference, making it a prominent subject in the realm of MOF glasses. Delving into this study, we explored the incorporation of silver ions into ZIF-62. The introduction of silver was observed to critically impact the melting behaviour of ZIF-62, with the benzimidazole ratio in the structure playing a pivotal role. At reduced benzimidazole ratios, ZIF-62 leaned towards forming ZIF-zni at lower temperatures, while higher ratios enabled a full transition into an amorphous state. Techniques such as THz-IR and solid-state NMR illuminated silver's interactions within the framework, especially with the benzimidazole ligand. Post thermal treatment, silver-doped ZIF-62 revealed accessible Ag nanoparticles, leading to superior gas separation performance in mixed-matrix membranes, particularly in CO₂ and hydrocarbon separation selectivity in comparison to pure ZIF-62 glass. A notable discovery was the Ag nanoparticles' capability to modify alkene selectivity based on their size. These revelations underscore the potential of silver-doped ZIF-62 in applications ranging from gas separation to antimicrobial films, suggesting its vast applicative possibilities.

Biography



Ruiqi Chen is currently pursuing a Ph.D. in Chemical Engineering at the University of Queensland (UQ), Australia. Having completed both his undergraduate and master's degrees at UQ, Ruiqi has amassed a solid academic background and a keen interest in innovative research within the Chemical Engineering field. His primary research lies into the application of Metal Organic Framework (MOF) membranes for gas separation, aiming to revolutionize efficiencies in this critical sector.

Sandra Kentish

Carbon Dioxide Capture – the Challenges Ahead

Sandra Kentish

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Carbon dioxide capture has been in operation within the petroleum industry for over 100 years, where it used to purify natural gas streams. The technology within this application is well established and cost effective. However there are many challenges to scale this technology to meet the need for Net Zero Emissions; and to apply it to other gas streams. This presentation will discuss the impact of CO₂ concentration and that of the impurities present in the gas stream. Direct air capture will be contrasted against that from cement factories and from the production of blue hydrogen. The work of my own group using both gas separation membranes and membrane contactors will be briefly described. Finally, some options for the integration of the capture operation with utilisation will be discussed.

Biography



Professor Sandra Kentish is a Redmond Barry Distinguished Professor at The University of Melbourne. She is a Project Leader within the ARC Hub for Digital Bioprocess Development, the Dairy Innovation Research Hub and within the Future Fuels CRC. She is a member of the Science, Health and Engineering Advisory Committee for EPA Victoria and a Board Member of the Bionics Institute. She was Head of the School of Chemical and Biomedical Engineering (2017-2022), Head of the Department of Chemical Engineering (2012-17) and the Discipline Leader in the CRC for Greenhouse Gas Technologies (CO2CRC) for Membrane Technology from 2003-2015. She was selected as one of Australia's Most Innovative Engineers by Engineers Australia in 2017 and as a Woman of Influence by the Australian Financial Review in 2018. She was elected to the Australian Academy of Technology and Engineering (ATSE) in 2019.

Sankar Bhattacharya

CO₂ conversion to methane – current status and the way forward

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The ever-increasing levels of atmospheric CO₂ call for its reduction and if possible, its valorisation to valuable fuels and chemicals. Methane is one such high-value fuel and an important hydrogen carrier. It is also the major component of natural gas which is currently transported around the world, and CO₂ methanation is much faster when compared to other hydrogenation reactions to hydrocarbons or alcohols. Thus, CO₂ valorisation to methane has been an area of development in the past few years. In methanation, choice of long-lasting and inexpensive catalyst is the key. This presentation summarises the current status worldwide at different scales and presents the path forward for development. We also present the key results from our own work where we examined the catalytic activity of 3D-printed metal monoliths loaded with iron impregnated ceria-zirconia mixed-oxide support on CO₂ conversion to methane was investigated between 300 and 500 °C under 1 bar and 20 bar pressure. The catalyst was characterised using TPR, XRD, SEM-EDX and in-situ DRIFTS. At 400 °C and atmospheric pressure, the catalyst wash-coated monoliths increased the methane yield by 3.5 times and doubled the CO₂ conversion compared to the same catalyst dispersed as a powder. Methane selectivity of 95.2% was obtained at 400 °C and 20 bars pressure. This is the highest methane selectivity recorded in the literature for CO₂ methanation using an iron catalyst. The catalyst loaded monoliths were stable over a continuous operation of 100 h at 500 °C and 20 bar. Such increased methane selectivity and yield combined with a long duration stability as well as an economic and easier synthesis process vouches for the great potential of catalyst loaded 3D monoliths for industrial application.

Biography



Professor Bhattacharya joined academia in 2009, having worked in industry for over twenty years in three different countries – in India on power plant design and commissioning, in France managing the Cleaner Fuels program at the International Energy Agency, in Australia as a Principal Process Engineer with Anglo Coal Australia and as a Principal Research Engineer with the Lignite CRC in Australia operating large pilot plants in Australia and the USA. At Monash University, Professor Bhattacharya's research areas include a) thermo-catalytic processing of wastes to liquid fuels, chemicals and hydrogen, gasification, b) rare earth metal recovery from eWastes and fly ash, c) conversion of biomass to high-value platform chemicals. He leads a group of 16 PhD students and a research fellow, having supervised 35 PhD students to completion. Professor Bhattacharya advises several governments, domestic and international, on energy issues. He holds three patents, edited three books, authored six book chapters and over 180 journal papers on energy, fuels and biochemicals. He is a Fellow of the Australian Institute of Energy

See Wee Chee

Operando Electron Microscopy of Electrocatalysts Transformations under CO₂ Electro-reduction Conditions

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Using renewable energy to power the chemical conversion of CO₂ back into needed high value hydrocarbons is a vital strategy for moving our society towards sustainable development. The electrochemical reduction of CO₂ (CO₂RR) is particularly appealing for such applications. However, we still lack a complete understanding of the catalyst descriptors which are needed to rationally design optimal catalysts with high selectivity and long-term stability for CO₂RR. Particularly, it is essential that we characterize the catalysts under reaction conditions. For example, Cu, the most attractive catalyst for CO₂RR due to its ability to directly produce hydrocarbons, can undergo significant restructuring and dissolution during reaction, but these new structures not necessarily preserved when the sample is removed from the reaction environment. In this talk, I will present the work in my group using *operando* liquid phase electron microscopy (LP-EM) to reveal the structural transformations that take place in catalysts under reaction conditions with a particular focus on CO₂RR¹⁻³. First, I will briefly cover the instrumentation advances that allowed us to conduct electrochemistry experiments within the vacuum of an electron microscope. Then, I will cover how we used the technique to study the restructuring of model Cu-based electrocatalysts under CO₂RR conditions and how we associated the restructuring with its impact on hydrocarbon selectivity. Lastly, I will briefly discuss our efforts at combining *operando* microscopy and spectroscopy.

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Biography



See Wee Chee is currently the group leader for liquid phase electron microscopy at the department of Interface Science in the Fritz Haber Institute (FHI) of the Max Planck Society. Since graduating with a PhD in Materials Science and Engineering from the University of Illinois at Urbana-Champaign, See Wee has worked extensively on using electron microscopy to visualize dynamic processes in liquids and gases. His group at the FHI focuses on capturing and understanding the transformations that take place in electrocatalysts under applied potential and in the electrolyte with liquid phase electron microscopy and other complementary techniques.

Shizhang Qiao

Electrocatalytic Refinery for Production of Fuels and Chemicals

Shizhang Qiao

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Compared to modern fossil fuel-based industrial refineries, the emerging electrocatalytic refinery (e-refinery) is a more sustainable and environmentally benign strategy to convert renewable feedstocks and energy sources to transportable fuels and value-added chemicals. E-refinery promisingly leads to defossilization, decarbonization, and decentralization of chemical industry. Specifically, powered by renewable electricity (e.g., solar, wind and hydro power), oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) can efficiently split water into green hydrogen and CO₂ reduction reaction (CRR) can convert CO₂ emissions to transportable fuels and commodity chemicals.

A crucial step in realizing this prospect is the knowledge-guided design of appropriate reactions and optimal electrocatalysts with high activity and selectivity for anticipated reaction pathways, which dominantly involve cleavage and formation of chemical bonds between H, O and C. In this presentation, I will talk about our recent progress in mechanism understanding and material innovation for some crucial electrocatalytic reactions (OER, HER, CRR, etc.), which are achieved by combining atomic-level material engineering, electrochemical evaluation, theoretical computations, and advanced *in situ* characterizations. A special emphasis is placed on the rational exploration of novel single-atom catalysts.

Biography



Dr. Shizhang Qiao is a Chair Professor at the School of Chemical Engineering and the founding Director of the Center for Materials in Energy and Catalysis (CMEC) at the University of Adelaide (UoA), Australia. His research expertise lies in nanostructured materials for electrocatalysis, photocatalysis, batteries, and other new energy technologies. He has co-authored 520 papers in refereed journals with 116,880 citation times, resulting in an h-index of 175. In recognition of his research achievements, Dr. Qiao has been awarded several prestigious awards, including inaugural ARC Industry Laureate Fellow (2023), the South Australian Scientist of the Year (2021), ARC Australian Laureate Fellow (2017), ExxonMobil Award (2016), and ARC Discovery Outstanding Researcher Award (DORA, 2013) among others. He is an elected Fellow of Australian Academy of Science (FAA), a Fellow of the International Institute of Chemical Engineers (FIChemE), the Royal Chemical Society (FRSC), and the Royal Australian Chemical Institute (FRACI CChem). Dr. Qiao is the Editor-in-Chief of *EES Catalysis* (RSC) and also recognized as a Clarivate Analytics Highly Cited Researcher (over 124 current ESI Top 1% highly cited papers) in three categories (Chemistry, Materials Science, Environment and Ecology).

Shuwen Yu

Thin film composite membranes with enhanced microporosity for gas separation

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The separation process owns a high energy consumption in industrial production (~ 50%), and the chemical separation cost accounts for more than 60% of the total production process[1]. Membrane separation has the advantages, such as high efficiency, energy saving and environmental friendliness, which plays an important role in chemical separation. Microporous materials, such as microporous polymers and metal organic frameworks (MOFs), which can simultaneously achieve efficient mass transfer and high efficiency separation, are the star materials for the preparation of membranes with high gas separation performance. However, both microporous polymer membranes and mixed matrix membranes based on MOFs still face many technical challenges. Specifically, the separation factor of the microporous polymer membrane is not high enough and the physical aging problem is serious. For mixed matrix membrane, the non-selective interface defect is easy to produce. Aiming at these technical problems, based on the composite membranes containing microporous materials, the thin film composite membranes with microporous structure[2, 3] and thin film nanocomposite membranes[4] including amine modified ZIF-8 (NH₂-ZIF-8) were prepared by interfacial polymerization, respectively. CO₂/N₂ and Kr/Xe pairs were used to simulate the capture processes of CO₂ and Kr. The gas separation performance and transfer mechanism of the membrane were investigated. The results show that the rich chemical cross-linking structure formed by interfacial polymerization plays an important role in improving the gas separation factor, preventing physical aging and improving the interface compatibility between MOFs and polymers. The thin film composite membranes prepared in this work have broad application prospects in CO₂ and Kr capture for power plant flue gases.

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Biography



Shuwen Yu received his PhD degree in Nanjing Tech University in 2019. He works in Suzhou University in China. Currently, he is working as a visiting postdoc at the University of Queensland under the supervision of Dr Jingwei Hou. His research mainly focuses on polymer and metal-organic framework (MOF) composite materials for membrane separation.

Steffen Jeschke

Challenges and Methods for Molecular Modelling of Electrode-Electrolyte Interfaces

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The electrode-electrolyte interface and electric double layer (EDL) that develops at this junction is pivotal in controlling interfacial chemical reactions. Understanding of the EDL has been repeatedly refined to include more complexity.^{1,2} The EDL differentiates between adsorbates in direct contact with the electrode and those that are separated by solvent molecules, termed the inner and outer Helmholtz planes (IHP, OHP), respectively. Modelling interfaces is challenging due to co-existing non-Faradic processes such as molecular and ionic ad-/desorption and EDL formation, and Faradaic processes involving electron- and proton-transfer reactions and associated localised changes in pH, charge distribution, potential, capacitance, and impedance. Structural and dynamic aspects of the EDL remain poorly understood, requiring experimental studies by advanced analytical techniques, and modelling of Faradaic and non-Faradaic processes to predict and design improved electrochemical devices such as CO₂ electrolyzers.³ Here, we summarise popular computational approaches to modelling the EDL, highlighting their strengths and weaknesses in the context of different applications. Advances in computing power and computational chemistry enable atomistic simulations of the EDL by density functional theory (DFT) and classical force-field methods, depending on the specific electrochemical applications and desired focus on IHP or OHP.⁴ In the electrochemical reduction of CO₂, determining intrinsic structure-performance relationships for the electrocatalyst surface (comprising one component of the EDL) is crucial.^{5,6} Related computational studies often use DFT approaches, such as the computational hydrogen-electrode or grand canonical ensemble-based methods, to predict the electronic properties of electrocatalyst surfaces, the interactions between reactants and electrodes in the IHP, and ultimately reaction dynamics.⁷

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Biography



Dr. Steffen Jeschke is a chemist with expertise in battery technologies and molecular modelling. He completed his PhD at the University Muenster in Germany, and did a Postdoc at Chalmers University in Sweden. He spent five years at RMIT University in Melbourne working with BASF SE, where he applied molecular modelling and machine learning to study corrosion inhibition. Currently, he is a Research Fellow at Griffith University working on catalytic biomass valorization.

Thi Kieu Oanh

Heterojunction photocatalysts for aqueous phase CO₂ reduction

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The United Nations Intergovernmental Panel on Climate Change (IPCC) has warned that rising CO₂ atmospheric levels will increase global temperature by >1.7°C by 2100.[1] Inspired by natural photosynthesis, the photocatalytic reduction of CO₂ offers an opportunity to mitigate CO₂ emissions and exploit a new chemical feedstock for the production of hydrocarbon fuels and chemicals.[2] However, current catalytic technologies suffer from poor solar-to-chemical efficiency due to inadequate light harvesting, rapid recombination of photoexcited e⁻-h⁺ charge carriers, or slow transport of these charge carrier to the catalyst surface. Heterojunctions formed between inorganic semiconductors are a promising solution to all these issues, broadening the spectral range of light adsorption and increasing charge carrier lifetime.[3] Here we describe the synthesis, characterisation and application of heterojunction photocatalysts containing UV (TiO₂) and visible (graphitic carbon nitride, g-C₃N₄) light absorbers, (**Figure 1**) for the aqueous phase photoreduction of CO₂ to CO, methane, methanol and formic acid. Photophysical properties, and charge carrier transport across the TiO₂/g-C₃N₄ interface are probed by photoluminescence, photocurrent and photoresistance measurements to aid the development of structure-reactivity relationships. Photoactivity and product selectivity are a strong function of charge carrier lifetime and valence/conduction band energies.[4] Possible avenues for quantum-chemical modelling of CO₂ photocatalytic reduction will also be reviewed.[5]

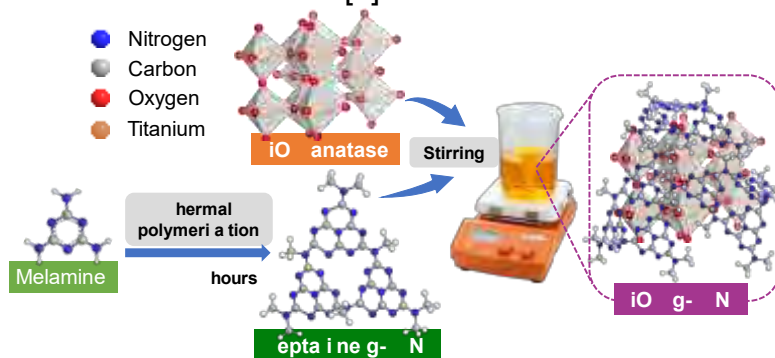


Figure 1. Synthesis of a heterojunction nanocomposite photocatalyst for CO₂ reduction.

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Biography

Thi Kieu Oanh is a Ph.D. student at Griffith University and received her Masters in Materials Science and Engineering from Gachon University, South Korea in 2022. Her researches focus on the design of heterojunction photocatalysts for application to CO₂ reduction and water splitting.

Timothy T. Duignan

Calculating activities with equivariant neural networks potentials

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Molecular dynamics (MD) can unveil a level of molecular scale detail that is impossible to access otherwise. For instance, many key structural, kinetic, and thermodynamic properties of electrolyte solutions cannot be measured experimentally but are key to understanding and modelling a huge range of biological and chemical systems where electrolytes play a critical role. A particularly important quantity is the activity coefficients which are key to determining chemical equilibria and reaction rates in solution. This is true for CO₂ capture and conversion which mainly occurs in electrolyte solution. Determining these properties with MD is constrained by an accuracy-efficiency trade-off. The combination of long-range electrostatic and complex short-range quantum mechanical forces means that simulating electrolyte solutions is particularly challenging. Here, we accurately and efficiently run accelerated MD of aqueous LiCl solution using both all-atom and coarse-grained equivariant neural network potentials (NNP). The training data is from a small set of first principle calculations using density corrected density functional theory (DC-DFT) on structures extracted from MD at a single concentration. Long-range electrostatics are treated with a continuum solvent model. The much larger and longer scales accessible with NNP-MD enables the computation activity coefficients and other key properties in agreement with experiment. Remarkably, we observe the formation of transient Li--Li pairs. We also demonstrate generalizability to lower concentrations, including infinite dilution and pure water. This approach can be scaled up to build a database of electrolyte solution properties, which will enable improved understanding of the many systems where these solutions are vitally important.

Biography



Dr Timothy T. Duignan is a Lecturer in Applied Maths and Physics at Griffith University and recently completed a Discovery Early Career Researcher Award in the School of Chemical Engineering at University of Queensland. He is working on the modelling and simulation of electrolyte solutions combining continuum solvent models, ab initio molecular dynamics and deep learning. He is focussed on developing these techniques for application to improving electrochemical energy storage and CO₂ capture and conversion. He completed his Ph.D. in the Applied Mathematics Department at the Australian National University in Canberra before carrying out postdoctoral research at Pacific Northwest National Laboratory in Washington State, USA.

Tom Rufford

Shockingly large volumes of materials may be required for large scale CO₂ electrolysis to make a dent in carbon emissions

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In this working paper I explore the scale of materials supply required for catalysts and membranes in electrolyzers for large scale CO₂ transformation. This paper builds on my presentation at the 2023 International Conference on Materials Innovation. The case study explored is the 3.5 million tonnes of CO_{2e} from Queensland's industrial processes^[1], that is non-electricity generating operations such as QNP, Boyne Smelter, Cement Australia. This analysis is informed by a previous technoeconomic analysis^[2], feasibility studies completed in student capstone design projects, and critical review of the recent literature. The critical materials analysed are the functional components in the anode, cathode, and membrane of an electrolyser to convert CO₂ to CO, with underlying assumptions that sufficient renewable energy infrastructure is available to power the process and that there is a ready market for the CO produced. Rough estimates in this analysis suggest 14 tonne of Ag nanoparticles are needed for the cathode, 7 tonnes of IrO₂ is needed for the anode, and something like 50 tonne of an ion exchange membrane is required. Key issues identified in this work will need to be addressed for very large-scale deployment of CO₂ electrolysis include choice of product, capacity for local electricity transmission to the site, supply of anode materials and ion-exchange membranes. Improving electrolyser stability and extending operating life also remains a significant challenge that will affect the overall costs and environmental impact of CO₂ electrolysis technologies when deployed at large-scales.

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<https://doi.org/10.26434/chemrxiv-2021-7chqx>

Biography



Tom Rufford is an Associate Professor in the UQ School of Chemical Engineering and a chief investigator in the ARC Centre of Excellence for Green Electrochemical Transformation of CO₂ (GETCO₂). Tom completed his BE and PhD degrees in Chemical Engineering at the University of Queensland in 2000 and 2009, respectively, with a few years spent working as a process engineering in an oil refinery between these degrees. His research interests include electrochemical processes for CO₂ conversion to valuable products, low emission steel production, gas process engineering, porous carbons, and solid-fluid interactions in coal seam gas reservoirs.

Tu Le

Machine Learning for Materials, a Journey from Artificial Intelligence to Intelligent Materials

Tu Le

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The design and synthesis of materials with useful, novel properties is one of the most active areas of contemporary science, generating a veritable explosion of scientific activity in areas such as biomaterials, cell and tissue engineering, organic photovoltaics and light-emitting materials, and nanomaterials for a myriad of medical and nonmedical applications. This new era of materials design and discovery covers many disciplines from chemistry and biology to physics and engineering. Conventionally, it takes at least 20 years to move a material from initial discovery to the marketplace. To accelerate the pace of novel materials discovery, computational methods such as artificial intelligent machine learning techniques can be used to construct predictive materials property models and allow rapid scanning of large chemical datasets to systematically identify attractive candidates for specific applications. This presentation will showcase recent studies on data-driven design of functional materials for a broad spectrum of applications such as drug delivery, antifouling materials, and CO₂ capturing materials.

Biography



Dr. Tu Le is a Senior Lecturer at the School of Engineering, RMIT University. She joined RMIT University in 2017, initially as the Vice Chancellor's Postdoctoral Fellow, then became a Lecturer in 2020. Prior to working at RMIT, she was a Postdoctoral Fellow and Research Scientist at CSIRO, from 2010 to 2016. Her research focuses on novel computational machine learning approaches to design and develop functional materials. The goal of these projects is to efficiently design fit-for-function materials by mapping the relationship between materials structures or processing conditions and their physicochemical properties. The application of these materials varies from drug delivery, anti-fouling coating, to hydraulic fluid for aircrafts. Dr. Le's research outcomes have been published in high impact journals such as Chemical Reviews, Chemical Society Reviews, Advanced Functional Materials, Nature Communications, Journal of the American Chemical Society and Small. Her research impact and contributions have also been recognized through many awards and grants, such as the Jacques-Emile Dubois award, CASS Foundation travel grant, and the joint Japanese Society for the Promotion of Science – Australian Academy of Science grant for attending the HOPE meeting with Nobel Laureates.

Venkata D. B. C. Dasireddy

Development of Ru-based catalysts for the CO₂ reduction : Power to Gas process

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Human-induced climate change and the resulting extreme weather events pose imminent existential risks, demanding a shift away from fossil fuels and the adoption of innovative strategies to curtail atmospheric CO₂. Catalytic technologies hold the potential to transform this crisis into an opportunity by harnessing CO₂ as a raw material to generate higher-value molecules in alignment with the 2030 UN Sustainable Development Goals¹. Although electrocatalysts show some promise for CO₂ conversion, such approaches still need to be scalable. In contrast, thermally driven Power-to-Gas (P2G) processes offer a promising solution^{1,2}. These processes involve converting renewable sources into hydrogen (H₂) and subsequent transformation into high-value, energy-intensive chemicals, such as methane, facilitated by active catalysts, which have become an effective solution for CO₂ reduction². Here, we conducted a comprehensive investigation into the hydrogenation of CO₂ using a series of Ru/ZrO₂ catalysts within a continuous flow microreactor and parallel, operando diffuse reflectance Fourier Transform infrared (DRIFTS) measurements to develop the structure-activity relationships^{3,4}. The pre-reduction of the catalyst significantly influenced the light-off temperature, enabling impressive CO₂ conversion rates (~85%) and high selectivity for CH₄ (>98%) at 300 °C. The pre-treatment process at 600 °C resulted in varying oxidation states of Ru, including Ru⁰, Ru³⁺, and Ru⁴⁺. Elevated reaction temperatures led to a decrease in CO₂ conversion due to methane decomposition into CO/CO₂ and the water gas shift reaction converting CO to CO₂. Operando DRIFTS analysis revealed the presence of co-existing (bi)carbonate, formate, and reactive intermediates, whose surface speciation depended on factors such as Ru particle size, support acidity, redox properties, and the reaction environment. Notably, high CO surface coverages were found to suppress CH₄ formation.

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Biography

Dr. Venkata D. B. C. Dasireddy received his Ph.D in Applied Chemistry in 2013 at the University of KwaZulu Natal, South Africa. His expertise lies mainly in heterogeneous catalysis for green chemistry applications, chemical (process) engineering, reactor design and activating of C-H bonds through heterogeneous catalysis. From 2015 to 2019, He worked as a researcher in European Horizon 2020 projects like MefCO₂ and FRESME, focussed on converting CO₂ to green methanol. He also worked as a Lecturer and Course Co-ordinator for the Master of Material Science and Engineering at the University of Newcastle from 2019-2021. He has published over 100 scientific research papers (52 as first author) and has a h-index > 30.

Wengang Huang

Intermarrying MOF glass and nanoconfined perovskite for photo-enzyme coupled CO₂ reduction

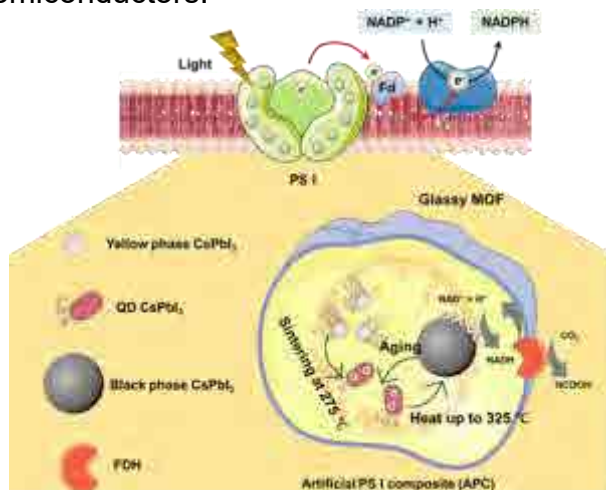
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Recently there has been a rapid development in perovskites and MOFs as photocatalysts. However, the low light-harvesting capability and ease of decomposition are still the main bottlenecks for MOFs and perovskite achieving desired photocatalytic ability. Herein, we introduce a new type of perovskite-impregnated MOF glass composite photocatalyst (a_gMOF-PVK) to mimic the properties of Photosystem I (PS I). The construction of a well-defined, intimate interface between the light-harvesting perovskite unit and MOF glass (a_gMOF) facilitated the photo-induced electron transfer for NADH regeneration with a high selectivity and productivity. The regenerated NADH can then be consumed by enzymes for CO₂ reduction, realizing artificial photosynthesis process. Moreover, perovskite's high temperature active phase γ -CsPbI₃, which spontaneously transforms to a non-perovskite phase (δ -CsPbI₃) upon cooling, is stabilized at room temperature in glassy a_gMOF. Due to the nanoconfined perovskite's shrinkage, this material exhibited red photoluminescence as an indication of aging after multiple cycles and regains 90% of its photocatalytic capacity after re-sintering. This work sheds light on effective electronic and energy bridging between perovskite nanoparticles and glassy semiconductors.



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Biography

Mr Wengang Huang is a Third-year PhD student in the School of Chemical Engineering, University of Queensland. He obtained his Master degree from Wuhan University, one of the Top 5 university in China before moving the Australia to pursue his PhD. His research projects mostly revolve around MOF and photocatalysis.

Xiaohe Tian

Bipolar Membrane Electrode Assembly for High-performance CO₂ Electrolysis

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CO₂ electrolysis represents a promising route for CO₂ utilisation to convert CO₂ to value-added products, such as carbon monoxide, ethylene and ethanol. The state-of-the-art CO₂ electrolyzers are constructed based on the membrane electrode assemblies, where a monopolar ion-exchange membrane (anion exchange or cation exchange membrane) is in direct contact with the cathode and anode. Due to the minimized gap between electrode and membrane, this cell configuration exhibits a low ohmic loss and simple cell structure. However, the use of monopolar membranes usually causes unstable pH profiles, which consequently lead to either carbonate formation on the cathode GDE blocking CO₂ transport and reaction efficiency or PGM-free catalysts dissociation in the acid local environment at the anode. One promising option to mitigate the critical issues is to use a bipolar membrane (BPM) in which hydroxide ions can be supplied to the anode and protons are supplied to the cathode. This poster will provide a critical review of BPMEA for CO₂ electrolysis. I will first discuss why BPMEA has the potential to stabilise electrolysis cells. Then I will summarise recent advances in improving cell performance by modulating the local reaction environment. We conclude the review by discussing the challenges and opportunities in reducing applied voltage and improving selectivity, such as the development of water dissociation catalysts for the bipolar membrane and acid-tolerant catalysts for CO₂ electrochemical reduction.

Biography



Xiaohe Tian is a PhD candidate in chemical engineering. He completed his bachelor's degree of chemical engineering from China University of Petroleum, China (2017) and his master's degree of Chemical Engineering from the University of Queensland, Australia (2019). His master thesis was conducted under the supervision of Prof. Thomas E. Rufford and Dr. Mengran Li. Here, he studied metal catalyst synthesis using electrochemical method for the reduction of CO₂. His finding of high-performance Cu-Sn catalyst for CO₂ electrolysis has been published at Applied Materials & Interfaces as a co-first author. In August 2023, he joined the University of Melbourne. His research focus is on developing a highly efficient, selective, and stable membrane electrode assembly (MEA) for CO₂ electrolysis through engineering approaches.

Yijiao Jiang

Heterogeneous Molecular Catalysis for Electrochemical CO₂ Reduction

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Electrochemical reduction of CO₂ to CO is a viable approach for sustainable manufacturing of industrial chemicals and consumer goods. Heterogeneous molecular catalysts proved to be one of the most active, selective, and cost-effective catalysts driving this process in an aqueous medium. Due to the low conductivity, their immobilization on the electrode surface is a key element of heterogeneous molecular catalysts that can be efficiently and easily recovered and reused in consecutive cycles. 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 the electrocatalytic performances in CO₂ electrochemical reduction compared to the noncovalent counterpart. However, the catalyst experienced a gradual loss of activity. To resolve this issue, a range of detailed mechanistic studies allow us to rational design a new type of catalyst imparting a significantly higher resistance to degradation. The resulting catalyst shows no sign of deactivation over the course of 300 h long electrolysis while maintaining a faradaic efficiency of CO over 95 %. The electron transfer from electrode onto the moiety plays an important role in overall redox kinetics. Our recently developed variable frequency square wave voltammetry (VF-SWV) allows direct 2D electrochemical mapping of charge migration and to explore the statistical distribution of the reaction rates. We believe this methodology could also be useful in other areas of electrochemical reactions.

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Biography



Associate Professor Yijiao Jiang is the Deputy Director of Macquarie University Research Centre for Transforming Energy Market and the Chair of Women in Engineering Committee. After completing her PhD at University of Stuttgart, she worked as postdoc at ETH Zürich. She was then awarded UNSW VC Fellowship and ARC DECRA. Her research interests focus on the development of heterogeneous catalytic systems for green chemical processes and renewable energy production. She has developed various in situ and operando techniques including NMR, EPR, IR, Raman, and photoelectrochemical spectroscopy. She is an Associate Editor of *Energy & Fuels* and *currently serves on the ARC College of Experts*.

Yong Zhao

Integrated CO₂ capture and electrolysis for CO production

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The electrochemical reduction of CO₂ represents a promising route for the direct generation of value-added chemicals and fuels, meanwhile, storing the renewable electricity. However, the current CO₂ electrolysis systems are mostly based on pure-CO₂ feed and gas-diffusion-electrode based electrolyzers, which suffers from energy- and capital-intensive CO₂ supply chains and thus is unsuitable for industrial application. Direct electrochemical conversion of the CO₂ capture solution avoids the energy-intensive CO₂ regeneration and purification steps and thus offers a solution to the large-scale CO₂ utilisation using renewable electricity. The challenges are the limited product selectivity and reaction rate in the system, which is caused by the extremely low concentration of reactant CO₂ (<30 mM) and CO₂RR kinetics at the catalytic interface.

Herein, we develop an integrated CO₂ capture-electrolysis system that comprises a composite CO₂ regeneration and diffusion layer to improve local CO₂ concentration in the vicinity of catalyst at the cathode. Employing a high-metal loading Ni-single-atom (4wt%) catalyst in this system, we achieve efficient production of CO at 150 mA cm⁻² with a CO selectivity of 70% from the simulated flue gas (10%) directly. By eliminating intensive upstream processes, our system achieves CO production with 30% less energy than the conventional CO₂ electrolysis combined with water electrolysis.

Biography



Dr. Yong Zhao is a Research Scientist at CSIRO Energy Centre. He obtained his PhD in Chemistry under the supervision of Prof. Gordon Wallace at University of Wollongong in 2019. From 2019 to 2022, Dr. Zhao worked as a research fellow at University of New South Wales, University of Sydney, and University of Toronto, respectively. His research has been focused on the electrochemical conversion of small molecules (e.g., CO₂, O₂, N₂, H₂O) with an emphasis on deciphering interfacial process and designing energy-efficient catalyst/reaction system. He has authorized 52 peer-reviewed articles including those in the top-tier journals like *Nat. Synth.*, *Nat. Comm.*, *Joule*, *Angew. Chem.* (over 2100 citations; h-index 24), addressed 16 invited talks (1 session chair), and been selected as “*Nano Research* Young Star Editor” and “J. Mater. Chem. A Emerging Investigator”. Since January 2023, Dr. Zhao has started the electrocatalysis lab and been leading multiple projects at the CSIRO Energy Center. He aims to develop innovative electrochemical carbon capture and conversion technologies that enable the efficient production of renewable carbon fuels from waste CO₂.

Yu Yang

Ligand-tuning copper in stable coordination polymer catalysts for selective C-C coupling

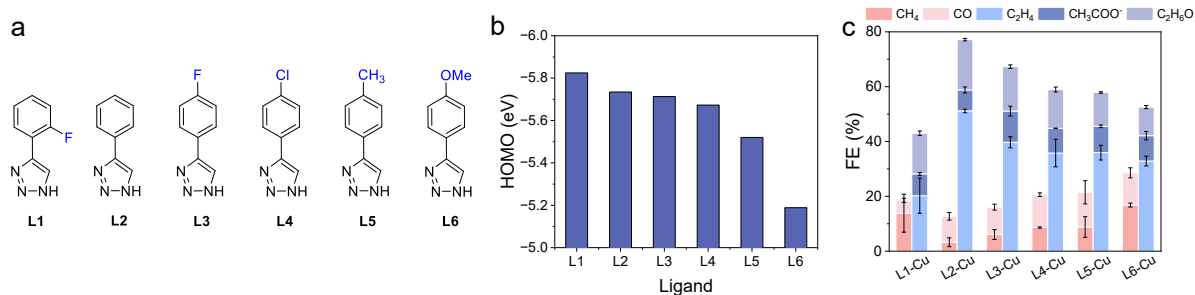
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Electroreduction of carbon dioxide (CO₂RR) provides a promising method to achieve net-zero carbon emissions. Cu-based catalysts have been extensively used in CO₂RR to efficiently produce valuable multicarbon products (C₂₊).¹ However, the control over product distribution is challenging due to multiple sites of heterogeneous catalysts.²

Single-site catalysts are advantageous for easier control over active sites at a molecular level, which can be applied to build the structure-function relationship.³ Here, I will show a series of stable single-site Cu coordination polymers (**L_n-Cu**, n=1 – 6) with similar coordination structures. The electron states of Cu were tuned by altering electron-donating ability of the ligands. The highest occupied molecular orbital energy of ligands—embodying the ligand-to-metal electron transfer capacity—was calculated to be negatively related to the Bader charges of Cu, which exhibited a volcano-shape trend relating to the C-C coupling efficiency. **L2-Cu** showed the highest C-C coupling efficiency with ethylene FE of 51% and C₂₊ FE of 77%. CO DRIFTS and DFT calculations demonstrated that the high C-C coupling efficiency derived from the modest Cu oxidation state which provided appropriate binding strength of *CO for *CO dimerization. Our work provides a perspective on regulating C-C coupling efficiency for higher C₂₊ selectivity by controllable tuning the electron state of Cu active sites.



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Biography



Yu Yang, is a PhD candidate in School of Chemical and Biomolecular Engineering, the University of Sydney. She is conducting research in the field of 'Electrochemical Carbon Dioxide/Carbon Monoxide Reduction' under the supervision of Dr. Fengwang Li. She is interested in the CO₂ capture and utilisation, specifically (bi)carbonate/carbamate conversion, and is trying to develop a carbon-efficient CO₂ conversion system.

Yuan Chen

Tailoring heterogeneous molecular Co–N–C catalysts

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Metal–nitrogen–carbon (M–N–C) single-atom catalysts show high catalytic activity for many important chemical reactions. However, understanding their intrinsic catalytic activity remains ambiguous because of the lack of well-defined atomic structure control. Here, we design heterogeneous molecular catalysts by anchoring metal-containing porphyrin molecules on carbon nanotubes to elucidate the intrinsic catalytic activity of metal centers in M–N–C catalysts. A pH-universal activity trend is discovered among six 3d transition metals for hydrogen peroxide (H₂O₂) synthesis, with Co having the highest catalytic activity. The difference in the binding energy of O₂^{*} and HOOH^{*} intermediates (E_{O₂^{*}} – E_{HOOH^{*}}) on single metal centers is a reliable thermodynamic descriptor to predict the catalytic activity of metal centers. We further show that the porphyrin β-substituents and the carbon substrate can modulate the catalytic activity of Co–N–C. An octafluoro-substituted Co–N–C catalyst exhibits >94% H₂O₂ selectivity and a high turnover frequency of 3.51 per second at an overpotential of 200 millivolts in an acid electrolyte. It can reach a maximum H₂O₂ productivity of 10.76 molH₂O₂ g_{cat}⁻¹ h⁻¹ in a two-electrode electrolyzer, delivering pure H₂O₂ solutions that can be used directly for water treatment and chemical production. We expect that this class of structurally defined heterogeneous molecular catalysts may be further applied to understand the activity of M–N–C catalysts for the electrochemical reduction of CO₂.

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Biography



Professor Chen received a bachelor's degree from Tsinghua University and a Ph.D. from Yale University. He is a professor at The University of Sydney. His research focuses on carbon materials and their sustainable energy and environmental applications, including batteries, supercapacitors, electrocatalysts, membranes, and antibacterial coatings. He is a fellow of the Royal Society of Chemistry and the Institution of Chemical Engineers. He is currently an editor for *Carbon* and *Journal of Alloys and Compounds*.

Yuting Zhuo

Optimising the flow behaviours in flow channels via CFD modelling to accelerate electrolyser performance

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Abstract

Anion exchange membrane (AEM) alkaline water electrolysers are pivotal in large-scale green hydrogen production, offering benefits from established alkaline electrolysis techniques, renewable energy integration, and the use of economical, non-precious electrocatalysts. Yet, research has predominantly concentrated on electrocatalyst innovation rather than electrolyser design, which is equally crucial for performance enhancement. This study reveals the significant impact of flow channel designs, such as single serpentine, parallel, and pin types, on AEM electrolyser efficiency. We employed a three-dimensional (3D) volume of fluid (VOF) computational fluid dynamics (CFD) model to simulate and analyze the two-phase flow dynamics, focusing on electrolyte and gas bubble mass transfer within these channels. A new design, termed 'Parpentine,' merges optimal electrolyte flow distribution, efficient bubble evacuation, and minimal pressure drop. The Parpentine design's effectiveness was validated experimentally using an operational AEM water electrolyser with Ni foam-based, and proprietary NiFe and NiMo electrodes. At a cell voltage of 2.5 V, we observed a hydrogen production efficiency increase ranging from 12.4% to 34.8% under 1 M and 5 M KOH conditions at ambient temperature. This study highlights the significance of using modelling method to refine the structure design of electrolysis systems, thereby boosting their performance. Furthermore, it emphasises the considerable promise that this method holds for advancing CO₂ capture and reduction technologies through the application of electrolysis systems.

Keywords: Electrolyser, flow channel design, two-phase flow behaviours, computational fluid dynamics (CFD), efficiency improvement.

Biography

Dr Yuting Zhuo is an ARC Industry Early Career Industry Fellow at the School of Chemical Engineering, UNSW. He completed his PhD at the University of New South Wales (UNSW) in 2020. His research focuses on the process modelling of clean energy production, storage, and applications.



Zeno R. Ramadhan

Stacking Fault in 3D Branched Ni Nanoparticles for Improved Catalytic Activity

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Stacking faults embedded in nanoparticles is one of the techniques to improve the catalytic activity of the reaction. Stacking faults induce the low coordination atom and significant lattice strain which is the key to improving electrocatalytic reaction by tuning the adsorption of reactant or intermediate. In nickel material, energy formation of *hexagonal close-packed (hcp)*-Ni, *face-centered cubic (fcc)*-Ni, and *hcp/fcc*-Ni is quite small and can occur in mixed phase of *hcp* and *fcc* in Ni materials. The fault of stacking in the mixed phase of *hcp* and *fcc* Ni is called stacking fault. Translating stacking fault density to activity can elucidate the relation between stacking fault and activity. The seeded growth gold core nickel branch was used to tune branch width by using different gold seed sizes under hydrogen gas. Increasing the branch width resulted in increasing the density of the stacking fault. Stacking faults can control the thermodynamics of Ni²⁺/Ni³⁺ oxidation, resulting in high activity for HMF oxidation.

Biography

Zeno R. Ramadhan is a Scientia Ph.D. Candidate in the School of Chemistry at UNSW. He graduated with a B.Eng. from Diponegoro University, Indonesia, in 2015 and obtained an M.Eng from Pukyong National University, South Korea, in 2018. His primary research interest revolves around solution-phase synthesis for tuning the active sites of transition metal-based materials, especially Co and Ni, through structural modification that encompass controlling crystal phases, grain boundaries, and compositions for catalytic applications.

Zhe Liu

Liquid state nanoionics: high-performance computing for novel physics and cross-scale models for engineering

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Dynamic ionic systems are the hidden engines of many electrochemical energy storage and conversion technologies. During dynamic working conditions, the systems are driven far from the equilibrium state. The interplay of multiple transport processes in the heterogeneous electrodes or at the electrolyte/electrode surfaces at their respective time and length scales leads to pronounced ion/electron spatiotemporal heterogeneity, which has enormous implications for functions and performances. Understanding and manipulating the transport and storage behaviour of ions and electrons inside or at the interface of the electrified nanoporous electrodes are essential to developing new systems and optimising existing ones for these energy technologies. However, the spatiotemporal evolution of ions/electrons is not well understood, which is a crucial bottleneck to bridging fundamental science with engineering applications. To address the challenge of lagging knowledge, the community calls for a paradigm shift from intuitive speculation to confirmed scientific knowledge, from trial-and-error serendipity to science-based design, and from qualitative modelling to quantitative prediction.

This presentation will overview our computational materials research for ion storage/transport in nanoporous materials in the past decade. This talk will start with recently discovered ion transport properties/phenomena in our graphene membrane platform with continuously tunable nanoslit size from 10nm down to 0.5nm and MOF/ZIF membranes with designable channel size and surface chemistry. This talk will review our high-performance computing study to reveal the underlying physical mechanisms, such as ion pairing regulated ion transport and dehydration and ion-wall interaction competition-induced ultra-high ion selectivity in MOF/ZIF channels. In the end, this talk will also introduce our efforts in developing methods for system-level device design, including continuum models, low-order nano-circuitry models, and machine learning.

Biography

Dr (Jefferson) Zhe Liu is an Australian Future Fellow, Professor of Computational Materials Engineering, and leader of the Integrated Computational Materials Engineering (ICME) consortium at The University of Melbourne. He got a PhD from the Materials Science and Engineering Department at Northwestern University in the US. After that, he spent two years as a postdoc research fellow at the National Renewable Energy Laboratory in the US. The research interests of Dr Zhe Liu's group are to develop/employ ICME methods for dynamic ionic systems in electrochemical energy storage and conversion and clean environment applications. Differing from the conventional research strategy in the ionics field that mainly deals with the ion transport problems at separated length scales, Liu's group are focusing on using integrated computational methods to translate the nanoscale ionic science to larger length scale applications by integrating digital models at different length scales, simulations with data science, and theory with experiments.

Zhijian Wan

A Scalable Material for the Deployment of Direct Air Capture

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The widespread implementation of direct air capture (DAC) faces significant obstacles due to the substantial costs associated with inefficient absorbent materials and high energy consumption. This study introduces an efficient absorbent that is a solid amine, and its CO₂ absorption performance was initially screened in a pure CO₂ environment and then compared with those commonly reported amine absorbents. In this study, other amine absorbents were diethanolamine (DEA) impregnated on various solid porous materials, such as silica (SiO₂), zeolite, activated carbon (AC) and polystyrene resin (poly-resin). The solid amine showed a high CO₂ uptake of 7.5 wt.%, slightly higher than that of the DEA/SiO₂ (7.3 wt.%) but significantly outperforming others, which was 5.3 wt.% for DEA/zeolite, 3.9 wt.% for DEA/AC and 3.1 wt.% for DEA/poly-resin. Furthermore, all the materials were subjected to accelerated ageing test conducted at 80 °C in air for 7 and 14 days. The solid amine incurred a 14.8% reduction in CO₂ uptake to 6.4 wt.% after one week and 18.6% to 6.1 wt.% after two weeks, still surpassing many pristine materials reported in the literature. In contrast, DEA/SiO₂ lost 25.3% of its CO₂ absorption capacity within the first week. The worst scenario was seen in the DEA/AC system, which had a 80% reduction in the first week. Moreover, when evaluated for DAC the solid amine demonstrated CO₂ uptake of 7.2 wt.%, double that of the DEA/SiO₂ (3.5 wt.%). More importantly, the CO₂ saturated solid amine can be regenerated at a low temperature of 80°C. This solid amine absorbent not only maintained high activity of amine for CO₂ absorption but also retained a solid form for ease of handling and regeneration, making it a promising candidate for commercial deployment of DAC.

Biography



Dr Zhijian Wan obtained his doctoral degree from The University of Western Australia. He is currently a research scientist at CSIRO, with primary focus on the development of environmentally sustainable and scalable absorbent materials tailored for CO₂ capture, specifically focussed on direct air capture. His research interests include CO₂ capture, CO₂ conversion and utilisation, clean energy and fuels, material science, hydrogen production, and waste recycling.

Zhiliang Wang

Dipole Moment Tuning in Semiconductor Photoelectrodes

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The charge separation and transfer (CST) in photoelectrodes is regarded as the most crucial step for efficient solar energy conversion via photoelectrocatalysis. To accelerate the CST process, it is important to create strong electric field to enhance band bending in the semiconductors. Dipole moment created by defects, or the intrinsic dipoles can be applied to induce an additional depolarized electric field, leading to improved driving force for CST. In our research, lattice distortion via lithiation process is created in semiconductor photoelectrodes, which leads to the formation of defect dipoles in the photoelectrode. It can lead to bulk electric field to facilitate the CST for water splitting. Further research based on ferroelectric photoelectrode BiFeO₃ shows that these intrinsic dipoles can also be tuned via external poling treatment, wherein the aligned dipole moment can lead to precise control of the band bending degree, leading to adjustable charge separation and transfer efficiency in the ferroelectric BiFeO₃ photoelectrode. These findings have displayed how the break of symmetry in localized microstructure can be tuned and finally affect the dynamics of charge carrier transfer via dipole moment. It can inspire the design of more effective solar energy conversion processes.

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Biography

Dr Zhiliang Wang is an ARC DECRA fellow in The University of Queensland. He has focused on renewable energy conversion processes, including water splitting, carbon dioxide fixation and methane conversion. He has accumulated rich experiences in the design of photocatalysts and photoelectrodes and achieved over 80 publications in highly ranked journals with over 6000 citations. He has been awarded with the J G Russell Award by the Australia Academy of Science, UQ Foundation of Research Excellent Award by UQ and other prizes.

Zixun Yu

Interfacial engineering of heterogeneous molecular electrocatalysts using ionic liquids

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We demonstrate a facile interfacial engineering strategy using a hydrophobic ionic liquid (IL, *i.e.*, [BMIM][NTf₂]) to boost the performance of a nitrogen coordinated single atom cobalt catalyst (*i.e.*, cobalt phthalocyanine (CoPc) supported on carbon nanotubes (CNTs)). We find a strong correlation between the oxygen reduction (ORR) performance of CoPc/CNT and the thickness of its IL coatings. Detailed characterisation revealed that a higher O₂ solubility (2.12×10^{-3} mol/L) in the IL compared to aqueous electrolytes provides a local O₂ enriched surface layer near active catalytic sites, enhancing the ORR thermodynamics. Further, the hydrophobic IL can efficiently repel the as-synthesised H₂O₂ molecules from the catalyst surface, preventing their fast decomposition to H₂O, resulting in improved H₂O₂ selectivity. Compared to CoPc/CNT without IL coatings, the catalyst with an optimal ~8 nm IL coating can deliver a nearly 4 times higher mass specific kinetic current density and 12.5% higher H₂O₂ selectivity up to 92%. In a two-electrode electrolyser test, the optimal catalyst exhibits an enhanced productivity of 3.71 mol_{H₂O₂} g_{cat}⁻¹ h⁻¹, and robust stability. This IL-based interfacial engineering strategy may also be extended to many other electrochemical processes such as carbon dioxide reduction reaction, by carefully tailoring the anion/cation types, thickness and hydrophobicity of IL coatings.

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Biography



Zixun Yu is a graduating Ph.D. student supervised by Dr. Li Wei and Prof. Yuan Chen at The University of Sydney. His research focuses on catalyst design and electrochemical techniques for oxygen, water and carbon dioxide electrocatalysis.

Zongping Shao

Development of functional oxide electrocatalysts for low-to-intermediate temperature CO₂ electrolysis

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Efficiently converting CO₂ into value-added fuels or chemicals is a significant target for reducing CO₂ emissions and achieving carbon neutrality, while electrochemical CO₂ conversion will play an important role in such conversion, where the electrodes determine large the activity and selectivity. Both room-temperature conversion of CO₂ to C₂ and high-temperature conversion of CO₂ (together with H₂O) to syngas are believed the most promising ways for CO₂ utilization in electrochemical processes. In particular, solid oxide electrolysis cells are a device where CO₂ reduction reaction (CO₂RR) performs with high efficiency and fast kinetics at high temperatures. Here, we demonstrate our past efforts in the development of perovskite-based functional oxide electrocatalysts for both low and high temperature conversion of CO₂ to value-added products. A novel cathode, Sr₂Fe_{1.4}Zn_{0.1}Mo_{0.5}O_{6-δ}, used in a La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-δ} electrolyte-supported single cell, shows a high current density of 2.74 A cm⁻² at 850 °C (1.6 V) and excellent durability when operated at a current density of -1.0 A cm⁻² at 750 °C. These findings can guide the developments of high-activity and stability catalysts for carbon capture and utilization.

Biography

Prof. Zongping Shao is a John Curtin Distinguished Professor at Curtin University, his main research involves electrochemical energy storage and conversion and environmental remediation based on catalytic ways. Up to now, he has published around more than 700 papers including 5 in Nature, 1 in Science and 2 in Nature Energy, 1 in Nature Catalysis and more than 10 in Nature Communications. He is a Clavrate Highly cited researcher in both the fields of Chemistry and Materials Sciences.