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ARC Centre of Excellence for
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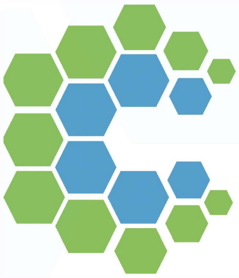
2024

International Conference on Advances in Carbon Science and Innovation

11-13 November
Sydney, Australia

Abstract Booklet



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Carbon photocatalysts for H_2 production and environmental remediation

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Persistent organic compounds, such as bisphenol A (BPA), chlorophenol and xenobiotics in aquatic systems pose serious threats to animal and human health. BPA is a precursor to epoxy resins and polycarbonate plastics, but a potent endocrine disruptor, while tetracycline discharge promotes antibiotic-resistant bacteria. Simple and energy efficient technologies are urgently sought to destroy such organic pollutants. Photocatalysts can harness solar energy to generate reactive oxygen species (ROS) from water and drive oxidative degradation of organics, however many such inorganic semiconductors are inefficient or prone to photocorrosion.

Here we discuss the use of carbons as components of low cost, scalable photocatalysts for the decomposition of organic pollutants in water under visible light.[1-3] Nanocomposites formed between e.g. graphene or reduced graphene oxide (RGO) and Earth abundant metal oxides create semiconductor heterojunctions that enhance charge carrier transport/lifetimes, and consequent concentration of ROS and activity for oxidative degradation (**Figure 1**).

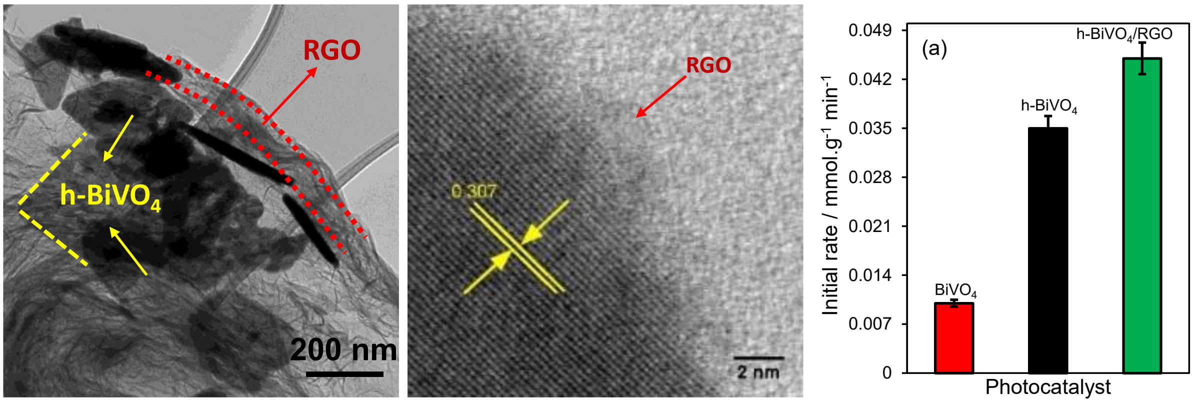

Figure 1. (a-b) HR-TEM images of hierarchical $BiVO_4$ plates/nanoparticles in contact with RGO, and (c) resulting catalytic performance for BPO degradation.

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Biography

Adam is Professor of Sustainable Chemistry at Griffith University, and previously held Chair appointments at Cardiff, Warwick, Monash, Aston and RMIT Universities. His research addresses the rational design of nanoengineered materials for energy and environmental applications. He is a Fellow of the Royal Society of Chemistry and Royal Australian Chemical Institute, Associate Fellow of the IChemE, Editor-in-Chief of M*aterials Today Chemistry*, and recipient of the 2011 McBain Medal, 2012 Beilby Medal and Prize, and 2023 RACI Welcome Award. Adam is a Chief Investigator on the ARC Centre of Excellence 'GETCO2'.

Defect Engineered Graphitic Carbon Nitride Nanosheets for Photocatalytic H_2O_2 production

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Graphitic carbon nitride (g-C_3N_4) is recognized as a promising photocatalyst for solar-driven H_2O_2 production, attributed to its tuneable electronic structure, and inherent visible light absorption[1, 2]. However, pristine g-C_3N_4 encounters fundamental challenges in photocatalysis, specifically limited photoexcitation and severe photocarrier recombination[3]. Introducing the nonmetals and/or metals into g-C_3N_4 to modify its electronic structure, enhance the charge transfer, and overcome the key challenges in oxygen reduction reactions has become pressing[4]. The lack of comprehensive understanding of local chemistry and doping over the structure of g-C_3N_4, reflected by conflicting reports in the literature[5, 6], has limited its application as high-performance catalysts.

Herein, we introduce a novel strategy for integrating metal sites coordinated with nonmetals in the g-C_3N_4 framework. Structural characterization via XRD, XPS, synchrotron X-ray absorption spectroscopy, and DFT calculations confirm the dispersed metal sites and their coordination with nonmetals. Various metals, such as Cu and Ni, coordinated with nonmetals like P, B, and S, have been doped into the g-C_3N_4 structure to investigate the effects of co-doping. The P-Ni co-doped g-C_3N_4 exhibited an H_2O_2 generation rate of 395 μmol g^{-1} h^{-1} and an apparent quantum efficiency of 11.2% at 420nm. This enhanced photocatalytic performance can be attributed to the nonmetal ligand coordination around the metal element, creating localized acceptor-like states near the Fermi energy and inhibiting the aggregation of metal atoms. The synergistic effect of co-doped nonmetal and metal improves the catalytic performance and material durability, making this modified g-C_3N_4 a promising platform for energy conversion applications.

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Adnan Ahmad obtained his Master's degree in Advanced Material Engineering from the National Textile University, Pakistan, where he focused on the fabrication and modification of carbon nanofibers for energy conversion applications, under the supervision of Prof. Muhammad Bilal Qadir. He is pursuing his Ph.D. in chemistry in Prof. Yun Liu's Functional Materials Research Group at the Research School of Chemistry, Australian National University. His research centers on synthesizing and modifying carbon-based two-dimensional materials, such as graphitic carbon nitride, for advanced photo-electrocatalytic applications, particularly in energy storage.

Computational Design of New Materials for Electronics, Energy and Environmental Applications

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Material properties are in-principle determined by electronic functionality. Now first-principles modelling can accurately calculate material electronic structure, allowing us to control electronic properties for illuminating “from the bottom up” structural, thermodynamics, and kinetic aspects of chemical and physical process, thus facilitating the rational design of new materials. In this presentation, we will choose some examples from our recent research showing how electronic functionality modulations via asymmetry, defect and ligand engineering to help the design of (i) a novel 2D multiferroic dual transition-metal dichalcogenide for electronics application [1]; (ii) optimal bimetal-doped $SrCoO_{3-\delta}$ perovskite as solid oxide fuel cell cathode for energy application [2]; (iii) a Cu-based metal–organic framework for the reduction of CO_2 into C2 products for environmental application [3].

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Biography

Aijun Du is currently a full professor at Queensland of 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 with 36,000 citations. He has been a Clarivate highly cited researcher since 2020.

Amorphous and Crystalline Nanoporous Carbon Nitrides with Tunable Nitrogen Contents for Clean Hydrogen Production

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Nanoporous Materials with ordered porous structures exhibit excellent surface features, including high specific surface area, large pore volume and uniform pore size distribution. Among the nanoporous materials with different functional elements, carbon nitride (CN) has emerged as the most researched material for catalytic applications due to the unique molecular structure with tunable visible range band gap, surface defect and basic sites, and nitrogen functionalities. These properties also offer anchoring capability with a large number of catalytically active sites, and provide opportunities for doping, hybridization and sensitization, etc. In this talk, I will present the development, capabilities, and current and future applications of multifunctional amorphous and crystalline nanoporous carbon nitride materials with different structures, band gaps, and nitrogen contents.[1-9] Much focus will be given on band gap engineering of these nanostructures through hybridization with other one and 2D nanomaterials, heteroatom doping and molecular tuning. I will also demonstrate how the chemical composition, structure, porosity and functionalization of these unique materials can be tuned.[3,10-11] In the last part of the talk, I will present the photocatalytic performance of these unique nanoporous carbon nitrides and their hybrids on water splitting to produce clean hydrogen from seawater. I will also demonstrate the utilization of this technology in converting seawater from different beaches along the coastal side of Australia.

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Bottom-up Hybrid Materials Design for Multifunctionality

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Abstract

There are ample of evidence of materials hybridization at scale, even in nature, yields optimal respond to specific functions. In structural materials, hierarchical materials hybridization accounting for defects or porosity would offer optimal performance at reduced materials mass. Similar thought process goes for other performance functionalities, thermal, electrical, dielectric, etc. Materials hybridization, core to materials design, offers unprecedented design space for optimizing device and system performance. The atomic-scale materials hybridization, analogous to pointwise material optimization, is arguably the ultimate materials morphology optimization goal. Advent of multiscale (atomic to continuum) materials modeling, associated with evolving reliable materials characterization techniques, appears convincingly promising for atomic-scale hybrid materials design and development. Success in integrating the atomic scale materials performance attributes to higher domain (both in temporal and spatial scale) with appropriate computational tools, such as density functional theory (DFT), Atomistic Molecular Dynamics (MD), tight-binding DFT, mesoscale Monte Carlo, Boltzmann Transport, Molecular Mechanics (MM), etc., shows early promise in this endeavor. In this presentation, examples of atomic scale hybrid material design unlocking specific performance goal, including concurrent multifunctional response, will be presented.

Metal Organic Framework Derived Carbon Materials for Carbon Dioxide Reduction Reactions

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Metal organic frameworks (MOFs) are coordination polymers belonging to the crystalline porous materials class. These frameworks, comprised of metal ion nodes connected through organic bridging ligands, can be tuned to accommodate different pore sizes by changing the geometry of the metal node or the size of organic linkers. However, due to their instability, most MOF frameworks are unsuitable for catalytic applications requiring high temperatures or pressures. A potential solution to these issues is MOF-derived materials obtained via a controlled thermal pyrolysis or partial combustion of parent MOFs, yielding catalytically active metallic nanoparticles embedded in a carbonaceous matrix. In this presentation, we report MOF-derived catalysts for converting carbon dioxide (CO_2) into value-added chemicals and fuels such as formic acid, acetic acid, polyoxymethylene dimethyl ethers and methanol. To complement the experimental study of CO_2 reduction, we employ large-scale reactive atomistic simulations to study the morphological transformation of metal encapsulated in MOF framework or bi-metallic MOFs. These reactive simulations allow us to address the limitations of contemporary computational methods to capture a reactive system's emergent properties. We show that tuning the MOF treatment temperature can lead to the formation of bimetallic nanoparticles, such as core-shell or alloy nanoparticles dispersed in a carbonaceous matrix. We identify and present sequential stages of the thermal transformation and the factors controlling them.

Presenter's Biography

Professor Akshat Tanksale, is a group leader in the Department of Chemical & Biological Engineering at Monash University, the Carbon Theme leader at the Woodside Monash Energy Partnership and the Deputy Director of ARC Research Hub for Carbon Utilisation and Recycling. He has pioneered work on Reactive Flash Volatilisation of biomass into hydrogen rich syngas, and CO_2 conversion into C_1-C_2 bulk chemicals such as syngas, formaldehyde and its derivatives, formic acid and acetic acid. He is a lead inventor on 2 patents on Reactive Flash Volatilisation, 3 patents on CO_2 conversion, in addition to 2 other patents on circular economy. His area of expertise is heterogeneous catalysis, nanoporous materials, reaction engineering and green chemistry. He currently leads projects with several industry partners on CO_2 capture and conversion, using heterogeneous and plasmonic catalysis. He is also one of the academic supervisors of the student team, Monash Carbon Capture and Conversion (MC^3) which recently won the US$250,000 XPrize Carbon Removal student competition.

Sustainable, highly porous carbon microspheres and their hydrogen storage performance

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Hydrogen holds the promise to a more sustainable energy future. However, its storage continues to be one of the main bottlenecks for its successful exploitation, especially in transportation. Hydrogen physisorption in porous materials, especially porous carbons, is considered as a viable route to achieve the required targets for vehicular hydrogen storage (US DOE targets for 2025 are 5.5 wt % and 40 g L^{-1}).[1] Nowadays, it is well established that adsorptive hydrogen storage is governed by the surface area/pore volume of the porous solid store, with micropores playing the leading role.[2] Consequently, research on hydrogen stores is targeting the development of highly microporous carbons (surface area > 2500 m^2 g^{-1}). Within this context, the sustainability of the synthesis route (attending energetic and chemical consumptions) is a key factor to ensure the development of a truly sustainable energy technology. Accordingly, in this work we present the synthesis of highly porous carbons from bio-based polymer microspheres by using a controlled physical activation process with non-toxic and cost-efficient CO_2. The polymer microspheres were obtained from biomass-based monomers, *i.e.*, phloroglucinol and glyoxylic acid, by using a microwave-assisted sol-gel methodology, which shortened significantly the synthesis time, reducing thereby the energy consumption. The control of the activation temperature coupled to the small particle size (spheres of *ca.* 1 μm) enabled a chemically control gasification process, leading to highly porous carbons with BET surface areas up to 3300 m^2 g^{-1} and pore volumes up to 1.6 cm^3 g^{-1}, yet possesing relatively narrow pore size distributions in the micro- to small mesopore region (< 3-3.5 nm). As a result, these materials have shown hydrogen uptakes up to 9.2 wt % (35 g L^{-1}) at 100 bar and -196 ºC.

Acknowledgements
This research was supported by the European Commission, Horizon Europe Framework Program, Call HORIZON-CL4-2021-RESILIENCE-01, Project MAST3RBOOST, GA 101058574.

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Presenter's Biography

Ana Fernández-Lera González is a PhD student in the Institute of Carbon Science and Technology (INCAR-CSIC). She is deeply passionate about Chemistry and Materials Science, which drove her to pursue a MSci degree in Materials Science. In 2023, she began her PhD focused on the development of highly porous carbons for hydrogen storage under the framework of a European project. She is comitted to the search for sustainable synthesis routes for this kind of materials that enable a truly sustainable future.

Synthesis and Applications of Multinuclear Metal Complexes with Controlled Metal-Metal Distances

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Across biological chemistry, synthetic chemistry and materials chemistry we find examples of enzymes, transition metal catalysts and catalytic materials in which multiple metal centres are found in the catalytic active sites, and catalytic mechanisms rely on the activity of multiple metals acting in concert.[1,2] In many cases, chemists do not have a good understanding of how the spatial and electronic relationship between the two metal sites, as well as the identity of the metals, plays into the activity and properties of the system.[3]

Our research team are interested in the design of dinucleating ligands that can house two metal centres in controlled coordination environments and at controlled metal-metal distances. This presentation will detail our work towards constructing such ligand systems and their transition metal complexes (Figure 1), including synthesis, characterisation, and applications of such systems, for example in catalytic hydrogenation and carbon dioxide electroreduction reactions.

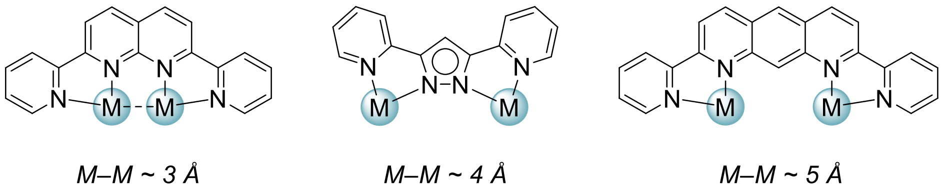

Figure 1. Example dinucleating ligand architectures and corresponding metal-metal distances.

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Presenter's Biography

Annie completed her PhD at the Australian National University, followed by postdoctoral appointments at the University of Bath, University of Oxford and University of Cambridge. She returned to ANU in 2019, where she is now a Senior Lecturer in the Research School of Chemistry and an Associate Investigator in the ARC Centre of Excellence for Carbon Science and Innovation. She has been the recipient of an ARC DECRA and the RACI Rita Cornforth Lectureship. Her research interests span synthetic inorganic and organometallic chemistry, catalysis, supramolecular chemistry and electrochemistry. Her research team develop synthetic methods to incorporate multiple metals into compounds, and study the impact this has on their properties and reactivity.

An electrochemical oscillator for harvesting near room temperature waste heat

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We present Soret effect-driven electrochemical devices that generate 1.02 V with a mere 10 °C temperature difference with the cold end at room temperature, i.e., a thermopower α of 102 mV °C $^{-1}$ - almost four times the record [*Adv Energy Mater* **9**, 1901085 (2019)]. We show that α depends not only on the electrolyte composition but also on the electrode porosity and microstructure, which has remained a neglected study area. Interestingly, our devices show novel voltage oscillations (unlike electrochemical oscillations observed previously, which were a result of either (a) stochastic single-molecule electrochemistry or (b) redox reactions) arising from an interplay between ionic diffusion and ionic migration within the electric double layer, indicating the potential for novel applications. A mere temperature difference of 13 °C across a module with four coin cells (connected electrically in series, thermally in parallel, and the cold end at room temperature) powered a calculator in real-time, which a commercial thermoelectric generator couldn't.

Presenter's Biography

Prof. Rao is the Robert A. Bowen Endowed Professor in the Department of Physics and Astronomy at Clemson University and the founding director of the Clemson Nanomaterials Institute. He is known for developing Raman spectroscopy as a versatile tool for characterizing carbon nanomaterials and developing liquid-injection-based synthesis methods for carbon nanotubes. His current research at Clemson University focuses on the many applications of carbon and other nanomaterials in energy harvesting and storage technologies. He has a strong record as a principal investigator on several projects funded by NSF, DOE, DOD, NIH, and private industries.

Carbonaceous Nanoparticle Dynamics in Ethylene Premixed Flame by Interfacing Monodisperse Model with Molecular Dynamics (MD) Simulations

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Combustion has been one of the most important engineered chemical reactions in industry. Aerosol methods, such as flame reactors have gained research interest due to their advantages for nanoparticle synthesis over traditional methods [1]. While flame-made Carbon Black is a versatile material widely used in various industries such as rubber manufacturing, Black Carbon, also called soot, is a harmful emission from fossil fuel combustion. Given that fossil fuels are expected to remain the primary energy source for transportation over the next 50 years, extensive research has focused on the negative impacts of soot emissions on health and the environment. A deeper understanding of combustion chemistry, however, is still missing especially during the early stages of soot formation. Such an understanding would not only aid in the development of cleaner combustion technologies but also provide valuable insights into the manufacturing process and the adjustment of chemical composition and final product properties of Carbon Black, which forms and grows in similar ways in flames.

Here, soot formation and growth are simulated by hierarchical modelling combining reactive molecular dynamics (MD) and a monodisperse particle dynamics model that tracks the soot particle number, carbon molar concentration, and particle surface area in ethylene premixed flames. The MD is used to determine the nucleation and surface growth rates of incipient soot based on a bond order formalism. These “ab initio” MD-obtained nucleation and surface growth rates are employed into a monodisperse particle dynamics model to describe the soot formation and further growth to large soot aggregates, allowing for linking process conditions with soot formation rate in flames. This connection between operating conditions and carbonaceous nanoparticle formation can be used to optimize the design of combustion systems to achieve important targets in emission regulations as well as functional properties of Carbon Black.

References:

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Presenter’s Biography Arash Fakharnezhad is a PhD student in the Department of Chemical Engineering at The University of Melbourne, specializing in combustion, aerosol science and multiscale modelling. His research focuses on multiscale modelling of formation and growth of carbon-based nanoparticles.

Nucleation Rate of Carbon Black Nanoparticles via Molecular Dynamics Simulations

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Carbon black is a versatile material widely used in various industries, including rubber manufacturing, pigment production, electronics and batteries, and as a reinforcing agent in polymers. Its nucleation rate, i.e., the rate of particle formation from gaseous precursors, plays a key role in the synthesis and application of carbon black, significantly affecting particle size distribution [1], chemical composition and final product properties [2]. In flame synthesis, nucleation is influenced by local temperature, gas composition, and residence time [3].

Here, chemical nucleation of carbon black is investigated during pyrolysis of n-heptane at high temperature (2200–2600 K) by reactive molecular dynamics (MD) simulations. The critical nucleus size is quantified by the free energy of formation at various temperatures and fuel concentrations. Increasing process temperature leads to smaller critical size, starting from 59±7 carbon atoms at 2200 K that decreases down to 33±3 carbon atoms at 2600 K (Fig. 1), while the fuel concentration hardly affects the carbon black critical size. The onset time of nucleation (induction time) decreases exponentially with temperature, consistent with previous shock tube pyrolysis experiments. The nucleation rate is obtained by the rate of formation of critical and supercritical hydrocarbon molecules. An Arrhenius-type relationship between the nucleation rate and the process temperature is proposed, exhibiting a 1st order dependency to the initial fuel concentration. The number density of carbon black nuclei derived by this nucleation rate is 4-5 orders of magnitude higher than that obtained by kinetic models for reactive polyaromatic hydrocarbon (PAH) dimerization. The present MD-derived nucleation rate can be readily used in particle dynamics models to account for process conditions on formation rate, without relying on detailed chemical reaction kinetic models.

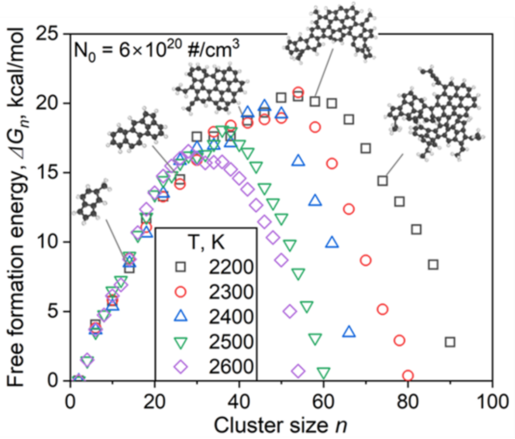

Fig. 1. Free energy, ΔG_n, of carbon black formation as a function of the cluster size, n, at 2200-2600 K for $N_0 = 6 \times 10^{20}$ #/cm^3. Insets show snapshots of clusters consisting of 13, 26, 44, 66 and 76 carbon atoms formed at 2200 K.

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Presenter's Biography Arash Fakharnezhad is a PhD student in the Department of Chemical Engineering at The University of Melbourne, specializing in combustion, aerosol science and multiscale modelling. His research focuses on multiscale modelling of formation and growth of carbon-based nanoparticles.

Carbon-based electrodes for alternative battery chemistries

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In the frame of this talk, I will present innovative methods for functionalising carbon-based nanomaterials, including 1D carbon nanotubes and 2D graphene nanosheets. The emphasis will be on alternative techniques for producing high-quality graphene nanosheets, highlighting the importance of scalable preparation of graphene structures for electrochemical applications. The discussion will illustrate how carbon nanomaterials and their composites can be employed to create diverse nanoscale topographies, leading to periodically functionalised structures ideal for multiple applications, including energy storage and conversion. I will also discuss recent developments in novel nanostructured 2D composites with improved properties, particularly for post-lithium-ion battery storage.

Presenter's Biography

Ashok is a Professor of Energy Storage at the University of Southern Queensland, Australia, and an Adjunct Honorary Professor at the University of Queensland. He is a carbon and energy expert and a former Chief Scientific Officer in graphene production and applications at a listed company. Currently, he leads the Clean Energy Research Group at UniSQ, focusing on materials for alternative energy storage technologies.

Fabrication of Three-Dimensional Boron-Doped Diamond Electrodes on SiC Scaffolds

Atsushi Otake[1], Irene Diaz-Herrezuelo[2], Kazuki Uchiyama[1], Andrea Fiorani[1], Manuel Belmonte[2], Yasuaki Einaga[1]
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Boron-doped diamond (BDD) has tremendous potential for use as a next-generation electrode material owing to its large potential window, small background current, superior biocompatibility, and surface functionalization capability. BDD is usually synthesized by chemical vapor deposition (CVD) on a two-dimensional substrate. Typical substrate materials for BDD deposition are Si or metal substrates. These 2D-BDD are commonly used for electrochemical analysis and electrochemical synthesis.

In the last few decades, additive manufacturing technology also known as 3D-printing has rapidly been progressed. 3D-printing produces three-dimensional solid objects with complex geometry from 3D-digital data, which are widely applied for rapid prototyping, chemical rectors, biomaterials, construction industries, automobile and aerospace applications. Recently, three-dimensional silicon carbide (3D-SiC) fabricated by a 3D-printing method was reported[1]. These 3D-SiC structures are known to provide three-dimensional reaction environment with enhanced fluid dynamics.

SiC is a suitable material for BDD deposition due to the chemical inertness, high thermal, mechanical and electrical stability. The 3D-SiC structures are expected to be used as micro-scaffold of 3D-BDD electrodes. The BDD coating on 3D-SiC is expected to exhibit advantages of micro-structured electrodes such as enlarged surface area, increased mass transfer, enhanced adsorption and exposing more active sites. In this study, we performed the deposition of BDD on the 3D-SiC micro-scaffold and discussed the electrical and electrochemical properties.

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Dr. Atsushi Otake is a Project Senior Assistant Professor at Keio University, Japan. After completing his master's degree at Keio University in 2001, he gained 20 years of experience at global chemical companies such as Mitsubishi, Dupont and Henkel. In 2009, he completed his Ph.D. studies in Tokyo University of Agriculture and Technology focusing on photoresisit materials and surface treatment solutions. Since 2021, he has been appointed to the CO_2 reduction project with diamond electrodes in Prof. Dr. Yasuaki Einaga's group at Keio University. His contributions have been globally recognized in the field of diamond electrochemistry.

Effects of Substrate Materials on the Electrochemical Properties of Boron-Doped Diamond Electrodes

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[2]Sensing System Research Center, National Institute of Advanced Industrial Science and Technology, 807-1 Shukumachi, Tosu, Saga 841-0052, Japan
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Boron-doped diamond (BDD) could serve as a next-generation electrode material owing to its large potential window, small background current, superior biocompatibility, and surface functionalization capability. BDD is typically synthesized by chemical vapor deposition (CVD) on substrates like single-crystalline Si substrates or metal substrates such as W, Nb, Mo, Ta, and Ti. The conductive mechanism of BDD has been studied in terms of surface termination and boron-doping levels, but reports on the effects of the substrate material are limited. In particular, the interfacial properties between BDD and its substrate have not been investigated yet.

BDD acts as a p-type extrinsic semiconductor because C atoms are replaced by B atoms with fewer valence electrons, thus making it an electron acceptor. Notably, metal/semiconductor junctions are formed at the BDD/metal substrate interface, whereas semiconductor heterojunctions are formed at the BDD/Si substrate interface. In metal/semiconductor junctions, Schottky barriers are possibly formed, whereas energy barriers, called band discontinuities, are possibly formed in semiconductor heterojunctions. In both cases, the interfacial energy barriers are normally accompanied by interfacial capacitances, which consequently influence the electron transfer at the BDD/substrate interface and the electrochemical properties of BDD electrodes. Therefore, selecting a suitable substrate material and understanding the electron-transfer mechanism at the interface are crucial.

In this study, the electrochemical behavior of BDD electrodes with different boron-doping levels (0.1% and 1.0% B/C ratios) synthesized on Si, W, Nb and Mo substrates were investigated. Potential band diagrams of BDD/substrate interface were proposed to explain different junction structure and electrochemical behaviors. Oxygen-terminated BDD with moderate boron-doping levels exhibited sluggish electron transfer induced by large capacitance generated at the BDD/Si interface. These findings provide a fundamental understanding of diamond electrochemistry and insights into the selection of suitable substrate materials for practical applications of BDD electrodes.

Dr. Atsushi Otake is a Project Senior Assistant Professor at Keio University, Japan. After completing his master's degree at Keio University in 2001, he gained 20 years of experience at global chemical companies such as Mitsubishi, Dupont and Henkel. In 2009, he completed his Ph.D. studies in Tokyo University of Agriculture and Technology focusing on photoresisit materials and surface treatment solutions. Since 2021, he has been appointed to the CO_2 reduction project with diamond electrodes in Prof. Dr. Yasuaki Einaga's group at Keio University. His contributions have been globally recognized in the field of diamond electrochemistry.

Keynote Presentation

Plasma Bio-Engineering: Advancing Biomimetic Devices, Biofabrication, and Nanomedicine

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Hunter Medical Research Institute (HMRI), New Lambton Heights, NSW 2305, Australia
School of Biomedical Engineering, University of Sydney, Sydney, NSW 2006, Australia
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The prevalence of implantable medical devices has witnessed a significant rise on a global scale, with an annual occurrence of hundreds of thousands of procedures. However, a substantial portion of these procedures experience complications, frequently associated with infections or insufficient integration with the host tissues. Implementing strategic surface functionalization with bio-instructive properties offers a viable approach to regulate biological reactions and direct the differentiation of stem cells through surface-attached biomolecules and hydrogels. Here, we showcase the remarkable capabilities of plasma bio-engineering techniques in crafting such instructive interfaces on a diverse array of materials. These materials span a spectrum of chemistries and geometries, including titanium, stainless steel, bioceramics, and polymers such as ePTFE and silk. Our findings provide evidence on the covalent immobilization of multifunctional protein layers, peptide molecules with preferred orientation, hydrogel coatings, and even silver nanoparticles on the plasma-engineered surfaces. These modifications lead to improved cellular responses and bolstered antimicrobial properties, validated for a broad range of biomedical engineering applications, from surface engineering of bone implantable devices to creating constructs for cartilage tissue regeneration. The plasma bio-engineering approach holds significant promise for developing the next generation of bioactive materials and interfaces, not only for biomedical implant applications but also for broader medical advancements.

Presenter’s Biography:

Dr. Behnam Akhavan, an Australian Research Council (ARC) DECRA Fellow and a Senior Lecturer of Biomedical Engineering at the University of Newcastle, heads the Plasma Bio-engineering Research Group at the School of Engineering and the Hunter Medical Research Institute (HMRI). Since obtaining his PhD in Advanced Manufacturing from the University of South Australia in 2015, he has held postdoctoral positions at the Max Planck Institute for Polymer Research and Fraunhofer Institute of Microtechnology in Germany, and the University of Sydney. Dr. Akhavan's pioneering work in plasma surface bio-engineering, published in over 70 journal articles, has led to innovative applications in healthcare and beyond. He is recognised by Engineers Australia as one of the nation’s Most Innovative Engineers.

Illuminating Gold(II): The Thermal and Photochemical Reactivity of Bridged Gold(II) Dimers

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Metal complexes exhibiting rare oxidation states attract significant interest due to their distinctive chemical and physical attributes. These entities are at the frontier of numerous catalytic and medical applications, including C-H activation, photochemical water splitting and anti-tumour therapies. A common strategy for stabilizing these atypical oxidation states is via bridging frameworks, which facilitate the creation of bimetallic species that possess a metal-metal bond. The $[Au_2X_2(\mu\text{-}ArPR_2)_2]$ family of complexes serves as a quintessential example of these species that was first synthesised around 30 years ago (Fig 1).[1,2] These complexes are composed of two Au(II) atoms and can be readily tuned by modifying their X-, Ar- and R-ligands/substituents.[1,2]

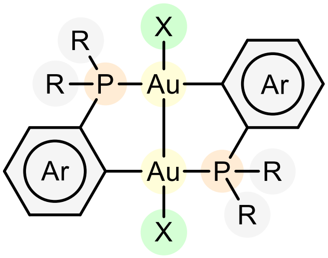

Fig 1: The structure of the $[Au_2X_2(\mu\text{-}ArPR_2)_2]$ family of complexes.

In this study, we utilise quantum mechanical (QM) and hybrid methodologies to explore the thermal and photochemical reactivity of these innovative complexes. We reveal new reaction pathways that elucidate the extraordinary chemical rearrangements these species undergo. These pathways help reconcile seemingly contradictory information regarding the stability of these materials. These insights solve a nearly 30-year-old puzzle and will pave the way for the design of novel bimetallic dimers for cutting-edge applications.

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Presenter's Biography

Benjamin Noble is an ARC DECRA Fellow within the School of Engineering at RMIT University. He graduated with a PhD in Physical Chemistry in 2017 from the Australian National University, under the supervision of Prof Michelle Coote. After undertaking a postdoctoral fellowship at ANU, he moved to RMIT University in 2019 to undertake a research fellowship. In 2022, he was awarded an ARC Discovery Early Career Research Award (DECRA) fellowship. His research interests include modelling polymerisation mechanisms, including photo- and electro-chemical processes and tranisiton metal/nanocluster catalysis.

Correlative Approach for Analyzing Porosity in Nuclear Graphite

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Nuclear grade graphites are high purity forms of graphite that have been engineered to resist the challenging environments in nuclear reactors. These graphites find application as neutron moderators and structural components in fission reactors, and neutron reflectors in developing fusion reactor designs. Importantly, the 3D microstructure of the graphite significantly affects the performance of the reactor and the ageing and degradation properties of the graphite itself. For example, the internal porosity of the graphite determines mechanical properties, corrosion resistance and its thermal transport properties. Thus, understanding the 3D microstructure of nuclear grade graphite is crucial for improving the performance of future nuclear reactors. However, identification and access of the region of interest (ROI) is a challenge in the adoption of 3D microstructure characterisation of graphites. To overcome this, a multi-scale Sample-in-Volume Analysis (SIVA) workflow has been developed. Microscale X-ray Microscopy (XRM) was deployed to non-destructively identify a ROI within a macroscopic sample volume. Unlike conventional microCT that relies on geometric magnification alone, XRM can image larger samples while maintaining highest resolution. The identified ROI can be accessed through massive material ablation using a femtosecond (fs) laser integrated on a Focused Ion Beam Scanning Electron Microscope (FIB-SEM). The workflow provides correlative means between the XRM and FIB-SEM stage to ensure coordinated access to the ROI. This enables 3D analysis via non-destructive synchrotron-calibre XRM with nanoscale resolution down to 50 nm. Elucidating the 3D microstructure of nuclear grade graphite is essential to understanding the performance and ageing characteristics of this critical material. This SIVA workflow provides valuable insights and data that can inform simulations to engineer novel forms of nuclear graphite with improved performance.

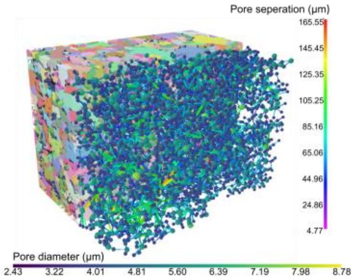

Figure 1: Intergranular graphite porosoity measured via X-Ray Microscopy (XRM)

Presenter's Biography

Dr. Bernd Schulz looks after the Materials Science sector at ZEISS Australia and New Zealand. He holds a PhD from UNSW Sydney and has over 10 years' experience as Materials Scientist within academic research and the manufacturing industry. This extensive experience has cultivated a deep understanding of microscopy techniques and their applications, equipping him to offer tailored solutions to a wide range of challenges.

Carbon based Functional Materials for Multivalent Metal Batteries

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The ever-increasing global energy demand and the depletion of finite fossil-fuel resources necessitate a proactive pursuit of sustainable energy alternatives and advanced energy storage technologies. Across various applications, from mobile electronics and electric vehicles to the broader power grid, the need for energy storage materials and devices exhibiting enduring cycling stability, high-energy density and power density remains unabated. In the quest for a sustainable energy future, alternative battery chemistries have emerged as promising candidates. These chemistries, based on multivalent elements such as Aluminium, Zinc, Iron, Magnesium, and Calcium, have attracted substantial attention owing to the relatively abundant supply of these elements and their potential for high-capacity energy storage. However, the intricacies of multivalent electrochemistry have introduced challenges and complexities that demand a thorough exploration. This presentation aims to shed light on functional materials designed to enable the realisation of competitive battery technologies, with a special focus on advancing materials for next-generation battery systems, e.g., Al-ion batteries. Additionally, this talk will provide a brief glimpse into our research endeavours, including collaborative efforts with industry partners, in the realm of Zn and Fe based redox flow battery technologies.

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Biography Dr Bin Luo is an ARC Future Fellow, Associate Professor & Group Leader in Australian Institute for Bioengineering and Nanotechnology (AIBN) at the University of Queensland (UQ). He received his doctoral degree in Physical Chemistry from National Centre for Nanoscience and Technology of China, University of Chinese Academy of Sciences in July 2013. Since joining UQ in 2014, he has worked as UQ Postdoctoral Research Fellow (2014-2018), ARC DECRA Fellow (2018-2021), and ARC Future Fellow & Group Leader (2021-) at AIBN. Dr Luo's research focuses on the design of new functional nanomaterials for energy storage application. He has contributed 5 edited book chapters, more than 130 original publications with total citation >13k and h-index of 56 (Google scholar). He is serving as Editorial Board/Young Advisory Board member of international journals including EcoMat, eScience and Catalysts.

Cabon-based materials for metal-air batteires

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Owing to the superior high energy density, metal air batteries (e.g. lithium–oxygen batteries and sodium–oxygen batteries) have been considered promising advanced battery systems to meet today’s stringent requirements as the power source for electric vehicles (EVs) and renewable energy storage. However, the development of metal air batteries is still constrained by several serious challenges, including uncontrolled side reactions, low energy efficiency and poor cycling life. The electrochemical performances of lithium/sodium–oxygen batteries await dramatic improvement in the design of porous oxygen cathodes, efficient electrocatalysts and stable metal anodes. Herein, we present the research outcomes from our group on carbon-based materials innovation for rechargeable metal air batteries. First, the family of metal air batteries will be introduced. Second, the design of porous carbon-based materials for high-performance air (oxygen) cathodes will be discussed. Third, facile and effective methods to enhance the electrochemical performance of lithium/sodium metal anodes will be presented, including three-dimensional current collector design and dual interface engineering on lithium/sodium metal anodes.

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Presenter’s Biography

Dr Bing Sun is a senior lecturer in School of Mathematical and Physical Sciences at University of Technology Sydney (UTS). He completed his Ph.D. at UTS in 2012 and then started his postdoctoral research in the Centre for Clean Energy Technology at UTS. His research interests focus on the development of next-generation battery materials and technology for high-energy-density batteries. He is the recipient of Australian Research Council (ARC) Discovery Early Career Researcher Award (2018) and ARC Future Fellowship (2022). Dr Sun has published more than 120 peer-reviewed articles, including *Nat. Energy.*, *Chem. Rev.*, *Joule*, *Chem. Soc. Rev.*, *Nat. Commun.*, *Sci. Adv.*, *Adv. Mater.*, *JACS*, *Angew Chem.*, etc. His research outputs have attracted 10,100 citations with an h-index of 59 (Web of Science).

Transforming Undesired Corrosion Products into a Nanoflake-Array Functional layer: A Gelatin-Assistant Modification Strategy for High Performance Zn Battery Anodes

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As corrosion products of Zn anodes in $ZnSO_4$ electrolytes, $Zn_4SO_4(OH)_6{\cdot}xH_2O$ with loose structure cannot suppress persistent side reactions but would increase the electrode polarization and induce dendrite growth, hindering the practical applications of Zn metal batteries. In this work, we build a functional layer on the Zn anode by a gelatin-assistant corrosion and low-temperature pyrolysis method. With the assistant of gelatin, undesired corrosion products were converted into uniform nanoflake array comprising ZnO coated by gelatin-derived carbon on Zn foil (denoted Zn@ZnO@GC). A series of in/ex situ tests and theoretical calculations reveal that the gelatin-derived carbons not only enhance the electron conductivity, facilitate Zn^{2+} desolvation, and boost transport/deposition kinetics, but also inhibit the occurrence of hydrogen evolution and corrosion reactions on the zincophilic Zn@ZnO@GC anode. Moreover, the 3D nanoflake array effectively homogenizes the current density and Zn^{2+} concentration, thus inhibiting the formation of dendrites. As a result, the symmetric cells using the Zn@ZnO@GC anodes exhibit superior cycling performance (over 7,000 h at 1 mA cm^{-2}/1 mAh cm^{-2} and over 2,000 h at 3 mA cm^{-2}/3 mAh cm^{-2}) and without short-circuiting even up to 25 mAh cm^{-2}. The Zn@ZnO@GC||NVO full cell delivers a high discharge capacity of 169 mAh g^{-1} and works stably for 5,000 cycles even with a limited N/P ratio of ~5.5, showing good application prospect.

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Presenter's Biography

Dr. Bing Wu received her B.S. degree in Materials Science and Engineering from Beijing University of Chemical Technology, Beijing, China, in 2021. She is currently pursuing her Ph.D. degree in Materials Science and Engineering with the School of Materials Science and Engineering, Beijing University of Chemical Technology, Beijing, China, as part of a direct Ph.D. program that began in 2021. Her research interests include the modification of zinc anodes for aqueous zinc-ion batteries, focusing on strategies to improve the performance and stability of zinc anodes through surface modification and structural optimization.

Efficient magnetic capture and valorization of micro(nano)plastics from water systems

Zhijie Chen, Bing-Jie Ni[*]
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Micro(nano)plastics (MNPs), defined as plastic particles < 5mm in size, have aroused increasing concerns as they pose threats to aquatic species and human beings. Removing MNPs from water bodies thus becomes an urgent issue.[1] Currently, a series of methods have been developed to extract MNPs from water bodies, such as froth flotation, adsorption, coagulation, filtration, and magnetic separation.[2] Among these methods, magnetic separation has attracted great interest due to its easy operation, high capacity, and less waste sludge.[3] However, conventional magnetic separation process has many limits, e.g., complicated and expensive magnetic seeds. In addition, most of current studies only focus on extracting MNPs from water, how to further manage the collected plastic waste is less explored. In this study, we have developed a green magnetic materials for efficient removal of MNPs from various water matrices. In addition, a novel valorization strategy is used to convert the collected plastic waste into efficient composite catalysts and to safely manage polyvinyl chloride-bearing plastics by fixing its Cl element. By developing cost-efficient magnetic materials for MNP removal and converting the plastic waste into valuable materials, this work would provide insights into the green and sustainable management of MNPs in global water systems.

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Presenter's Biography

Professor Bing-Jie Ni is an ARC Future Fellow and full professor at UNSW Water Research Centre. He has been working in the field of environmental technology and waste management, focusing on the integration of these disciplines to develop innovative and sustainable technological solutions to achieve high-levels of pollutant removal with minimised carbon emissions.

In situ Spectrometric Characterization for Carbon-based Electrocatalysis

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Carbon-based electrocatalysis is a cutting-edge field that harnesses the unique properties of carbon to enhance the efficiency and sustainability of electrocatalytic processes, paving the way for greener technologies and renewable energy solutions. *In situ* spectrometric characterization plays a crucial role in researching the mechanisms of carbon-based electrocatalysis, particularly through techniques such as *in situ* FT-IR and *in situ* Raman spectroscopy.

In situ FT-IR enables the monitoring of reactant adsorption and intermediate species, providing valuable insights into catalytic mechanisms and the influence of environmental conditions on catalyst performance. Meanwhile, Raman spectroscopy offers insights into the structural properties of catalysts, especially through the analysis of the D and G bands, which indicate disorder and graphitic content. By integrating these techniques, we aim to elucidate the relationship between structural characteristics and electrocatalytic activity, ultimately enhancing the design and optimization of carbon-based materials for various electrochemical applications.

For instance, *in situ* Raman spectroscopy can reveal the pathway of urea oxidation(Fig.1), while *in situ* FT-IR can probe intermediates in water oxidation, indicating that the O-O bond facilitates a multi-site mechanism (Fig.2). Additionally, *in situ* FT-IR can detect the S_3 radical, which is instrumental in developing high-energy lithium-sulfur batteries (Fig. 3).

In summary, *in situ* spectrometric characterization is essential for understanding the catalytic mechanisms of carbon-based electrocatalysis. It provides real-time insights into the changes occurring during electrochemical reactions, enabling the optimization of electrocatalysts and supporting the advancement of sustainable energy solutions.

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Presenter's Biography
Bingliang Wang is a PhD candidate of Univerisity of New South Wales, under the supervision of Prof. Liming Dai. He obtained his Master degree from Fudan Univeriusty, where he was supervised by Prof. Yongyao Xia. His research primarily focuses on electrochemistry, including electrocatalysis, *in situ* characterization, and battery technologies.

Exploring Direct Electrochemical Fischer-Tropsch Synthesis of C_1-C_7 Hydrocarbons via perimeter engineering of Au-$SrTiO_3$ catalyst

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Traditionally, Fischer-Tropsch (FT) synthesis is performed using thermal catalysts and syngas (CO and H_2) under high-pressure and high-temperature conditions to produce hydrocarbons. However, this study introduces an approach that relies on the electrochemical (EC) FT synthesis under ambient conditions [1]. A series of C_nH_{2n+2}, C_nH_{2n} hydrocarbons (n=1-7) was successfully produced over Au nanoparticle-loaded strontium titanate ($SrTiO_3$) nanostructures grown on rutile (TiO_2) supported on Ti. Au(1.0 nm)-$SrTiO_3$ shows the best interface formation, with the highest Faradaic efficiency for C_{2+} hydrocarbons. The optimal geometry of Au(1.0 nm)-$SrTiO_3$ and its catalytic activity were studied by a machine learning global optimization that leverages an on-the-fly surrogate Gaussian process regression model and an evolutionary algorithm [2]. The hydrogen weight distribution analysis and density functional theory calculations reveal that the direct EC-FT process proceeds via a C-C coupling chain growth reaction at the Au-$SrTiO_3$ interface [3]. The robust combination of experimental and computational findings reveals that optimum conditions and mechanisms for producing surface hydrogenation and C-C coupling polymerization, initiated by surface *CO and *H, are achieved by controlling the undercoordinated Au at the perimeter sites of supported Au nanoparticles. This EC-FT process opens a promising avenue for the direct conversion of CO_2 and H_2O into value-added long-chain hydrocarbons.

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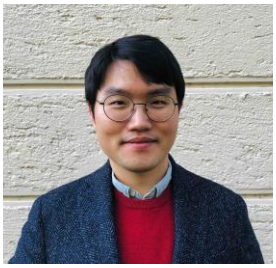

Prof. Chang Woo Myung is currently an Assistant Professor in Department of Energy Science at Sungkyunkwan University. He earned his B.S. and M.S. from Pohang University of Science and Technology (POSTECH) and his Ph.D. from the Ulsan National Institute of Science and Technology (UNIST) in 2019. He furthered his research as a postdoctoral fellow at ETH Zurich/USI and University of Cambridge. He served as an Assistant Professor in Department of Chemistry at Chungnam National University. His primary research focuses on the advancement of Bayesian machine learning potentials, first-principles simulations of complex energy materials, and development of quantum computing algorithms.

The frontier innovations of carbon-based energy conversion/storages

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The demands for sustainable alternative clean energy sources have been dramatically increased. Porous carbon electrodes play a critical role in the enhancement of energy conversion efficiency of devices. In particular, the dimensions and pore structure can significantly affect electrocatalytic performance toward energy conversions/storages. Different synthetic approaches are presented for unique 0-, 1-, 2-, 3-dimensional and hierarchical structured carbons, while rationally tailoring a porous networked structures for deeper effective depth, low polarization, high mass transport rate and low solid phase resistance and low interfacial resistance. Size-catalytic effects are used to greatly limit the shuttle effects for high-performance Li-S and Na-S batteries. Methods to delicately designed staired pyrolysis process for deriving rational pore structured carbon from bio-mass are presented. The mechanisms of dimension and pore sizes carbon to enhance the electrocatalytic performance will be discussed. This talk will mainly present our research works on the development of advanced porous carbon electrodes for various applications including batteries, solar cells, biofuel cells and supercapacitors.

Presenter’s Biography

Professor Li, Member of the European Academy of Sciences, Fellow of the American Institute for Medical and Biological Engineering, National high-level specially appointed experts, and a renowned overseas teacher recognized by the Ministry of Education. He is currently the Dean of the School of Materials Science and Engineering at Suzhou University of Science and Technology. He served as the founding Chair of the Materials and Energy Department at Southwest University and the first Director of the Chongqing Key Laboratory of Clean Energy Materials and Technology. He also served as a tenured full professor and head of the Department of Bioengineering at Nanyang Technological University in Singapore, as well as a member of the Science Advisory Committee and Chief Scientist at Motorola Inc. in the United States.Professor Li has made a series of pioneering works in the fields of advanced functional materials, biosensors and chips, green energy, especially power/energy storage batteries. He has over 300 patents from the United States, Singapore, and China, and has commercialized over 50 patents in China. He has commercialized and developed subcellular disease diagnosis technology and industrialized high-performance and low-cost cathode materials, biochar, and supercapacitors for new energies such as lithium iron phosphate batteries. The output value has exceeded 10 billion yuan. He has published over 900 scientific papers, including Nature Mater, Nature Energy, Nature Comm, JACS, Phys Rev Let, Angel Chem, Adv Mater, etc. The papers have been cited over 60000 times with an H-factor of 110. He has won the 2nd Class of China National Technology Innovation Award, the second prize of the Invention and Innovation Award, the second prize of the Chinese Medical Science and Technology Award, the highest scientific and technological award for outstanding inventions from Motorola in the United States, the Nanyang Research and Innovation Award from Singapore, the Innovation Talent Contribution Award from the Chinese Overseas Chinese Community, the Chongqing Friendship Award, and the Suzhou Honorary Citizen Award. He currently serves as an editor or consultant for several internationally renowned journals, including Joule and Nanoscale, and as the editor in chief of Materials Reports: Energy.Professor Li has provided guidance over 70 doctoral students and over 120 master's students. He has established extensive collaborations with research institutes and enterprises in countries such as Singapore, Australia, UK，France and South Korea.

The Interface Design of Graphdiyne for Electrochemical Energy Storage

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The rapid advancements of intelligent and multifunctional electronics have raised a significant challenge for the design of novel electrochemical energy storage systems integrated with functionalities of battery and smart conversion. Here, we developed a facile way to integrate an intelligent solid Mg-moisture battery (SMB) with simple structure, which can exhibit continuous humidity and solar-light dual responsive. The SMB was composed only by directly growing graphdiyne nanoarray on melamine sponge as cathode (GDY/MS) and Mg foil, free of additional electrolytes and separators, which greatly simplified the configuration of battery. As a multifunction cathode, GDY/MS integrates multiple functions including trapping and transferring water molecules, catalyzing HER, capturing, and utilizing solar energy. The GSMB shows a significant positive correlation between open circuit potential (OCP) and humidity. With the continuous decline of humidity, the OCP also decreases. Such GSMB can be applied as self-power humidity monitor, showing an ultrafast response time. The natural band gap of GDY makes it further as photoelectrode to capture light and generate photoelectrons, thus improving the hydrogen evolution reaction kinetics and enhancing output potential. This simple and efficient battery made method represents the future development direction of self-power supply equipment, intelligent electronic devices and intelligent battery integrated.

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Presenter's Biography

Changshui Huang is the Professor of chemistry and materials in the Institute of Chemistry, Chinese Academy of Sciences. He received his Ph.D. in University of Chinese Academy of Science, under the supervision of Prof. Yuliang Li. He has been the postdoc at the University of Wisconsin-Madison. After that he joined as the Professor of Chemistry and materials. Currently, his research area focused on the synthesis and application of graphdiyne based carbon materials for energy storage and catalysis. He has published over 160 papers on *Chem. Rev.*, *J. Am. Chem. Soc.*, *Sic. Adv.*, *Nat. Commun.*, *Angew. Chem. Int. Ed.* and so on. He is the recipient of Outstanding Science and Technology Achievement Prize of the Chinese Academy of Sciences for 2021. He services as the editorial board of academic journals for the journal of *Acta Physico-Chimica Sinica*, *eScience*, *Chinese Chemical Letters*.

The role of electrocatalytic materials in metal||sulfur batteries

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The slow surface-interface reaction in sulfur cathodes is the key to restricting practical applications of the metal-sulfur batteries. Applying catalysts in sulfur cathodes can significantly improve the surface-interface reaction efficiencies and thus improve battery performance. We mainly focused on developing catalysts and the mechanism of interfacial reactions in sulfur cathodes. It is revealed that sodium sulfide electrodeposition is the rate-determining step and demonstrated the significant impact of sodium disulfide dissociation energy barrier on the electrodeposition efficiency. We also introduced nitrogen-doped carbon catalysts loaded with metal single atoms in potassium-sulfur batteries, demonstrating that the synergistic effect of the metal sites and nitrogen sites improves the activities of the catalysts.

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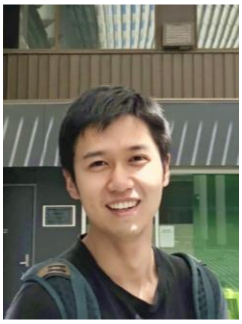
Presenter's Biography

Chao Ye received his PhD degree in 2020 from Prof. Shi-Zhang Qiao's group at the University of Adelaide, Australia. Now he works as a DECRA fellow at the University of Adelaide, Australia. As an early career researcher, he demonstrated an exceptional track record, reflected by the publication of 40 refereed papers in peer-reviewed journals, including papers as the first author, including: Nat. Commun., J. Am. Chem. Soc., Angew. Chem. Int. Ed., Adv. Mater., Matter, Adv. Energy Mater., Adv. Funct. Mater., Chem Catalysis, etc. His research interests are focused on energy storage and conversion such as metal-sulfur batteries and aqueous Zn-ion batteries.



Challenges and Opportunities for Single-Atom Electrocatalysts: From Lab-Scale Research to Potential Industry-Level Applications

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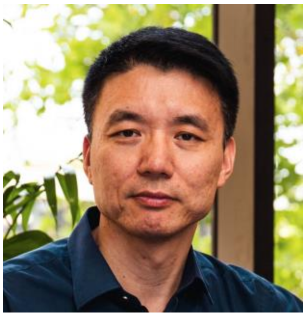
Single-atom electrocatalysts (SACs) are a class of promising materials for driving electrochemical energy conversion reactions due to their intrinsic advantages, including maximum metal utilization, well-defined active structures, and strong interface effects. However, SACs have not reached full commercialization for broad industrial applications. In this presentation, I summarise our progress in the design of efficient single-atom catalysts with advanced metal sites, novel coordination environments, porous substrates, and synthesis routes for electrochemical reactions such as water splitting, CO_2 reduction reactions and oxygen reduction reactions in hydrogen fuel cells. I will highlight the current challenges and opportunities for increasing intrinsic activity of metal sites, enhancing the utilization of metal sites, improving the stability, optimizing the local environment, developing new fabrication techniques, leveraging insights from theoretical studies, and expanding potential industrial applications.

Presenter's Biography



Prof 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. Prof Zhao received his PhD with an excellence award from Northwest University, then completed postdoctoral research at University of Oldenburg and Monash University, before starting his independent career in UNSW in 2010. He is currently the Deputy Director and Theme Leader of the ARC Training Centre for the Global Hydrogen Economy, the Deputy Research Chair, Flagship Program Director of the ARC Centre of Excellence on Green Electrochemical Transformation of Carbon Dioxide, and the past Chair of the Electrochemistry Division Royal Australian Chemical Institute (RACI). Prof Zhao is a Highly Cited Researcher and has received numerous awards including recently the R.H. Stokes Medal, the most distinguished award for Australian electrochemists. He is the elected Fellow of Royal Society of Chemistry (FRSC), Fellow of RACI (FRACI) and Fellow of Royal Society of New South Wales (FRSN). Prof Zhao is interested in discovering novel electrochemical methods and materials for applications in water splitting, hydrogen fuel cells, CO_2 reduction, aqueous batteries, and sensors. He has published more than 300 high impact research papers, and holds 16 families of patent of which 10 have been commercialised.

Carbon Fibre-based Structural Battery with Dual-Phase Solid Electrolytes

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Structural batteries are an innovative class of energy storage devices that integrate both structural load carrying capacity and energy storage into a single system. This dual functionality offers significant advantages, particularly in industries where weight and space optimization are crucial, such as electric vehicles (EVs) and fully electrical aircraft. Recent examples include integration of the 85 kWh battery pack into a structural frame in Tesla Model S, which makes up approximately 25% of the vehicle's total weight [1]. By integrating the battery directly into structural components, such as carbon fibre reinforced polymers, structural batteries can significantly reduce overall weight by eliminating the need for a battery pack, leading to increased energy efficiency, extended range, and improved performance [2]. However, existing structural batteries suffer from low energy density compared to conventional batteries due to the low ionic conductivity of solid-state electrolyte of high mechanical strength and stiffness. This issue arises from low ion conduction within the solid electrolyte and at the interface between the electrode and electrolyte [3].

In this study, we present a novel carbon fibre-based structural battery that integrates the active electrode materials of lithium-ion battery (i,e., lithium iron-phosphate and lithium titanoxid) into the carbon fibre fabrics along with a dual phase solid electrolyte [4]. The dual-phase electrolyte comprises a bi-continuous network of polymer matrix and ionic liquid (IL), along with surface functionalization to optimize the interface between the structural electrodes and the electrolyte. This configuration enhances ion conduction efficiency and mechanical robustness, which are crucial factors for maintaining the structural integrity and electrochemical performance of the battery.

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Presenter's Biography

Chun Hui Wang is a Scientia Professor and the Head of School of Mechanical and Manufacturing Engineering at the University of New South Wales (UNSW), Australia. He leads a research team focused on multifunctional composites for extreme environment applications. As the Director of the ARC Research Hub for Connected Sensors for Health, he leads a team of around 60 researchers in developing and deploying wearable sensors for human health monitoring and preventative healthcare.

Basic research on key technology and materials of off-grid produced green hydrogen

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Green hydrogen is an important part of the future energy system but its poor economy hinders the large-scale application. To systematically combine wind/solar-generated electricity, power device, and alkaline electrolyzers into an integrated system is to a feasible strategy to realize a full off-grid green hydrogen production. We present our recent progress on the development of the integrated off-grid green hydrogen production. The first progress is to upgrading the core material of power device based on silicon, which can efficiently track the maximum power point of the fluctuating electricity power from wind/solar, leading to ehanced efficiency. The second progress is to develop a general system of the capacity ratio of the green electricity and electrolyzer, which is a key factor to ensure the national and regional adaptability of the full off-grid system. The third progress is to develop non-precious Ni-based electrocatalysts and functional composite diaphragm, which is further combined with the new support structure and integrated electrode assembly, eventually building high-performance alkaline electrolyzers. In the integrated system, the electrolyzers can operate dynamically in the range of 20%-110% of rated load with energy consumption of $\leqslant$ 4.1 kW·h/Nm^3, and can match the fluctuating characteristics of green electricity. The key operating parameters and meteorological data of the whole system have been recorded in real time and monitored remotely, and the overall energy efficiency of the system under actual working conditions and its fluctuation with the climate are calculated, providing theoretical guidance and technical support for low-cost and large-scale green hydrogen production.

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Presenter's Biography

Prof. Chunxian Guo works as Professor and Executive Vice Dean at the School of Materials Science and Engineering, Suzhou University of Science and Technology. He obtained his Ph.D degree from School of Chemical & Biomedical Engineering, Nanyang Technological University (Singapore) in Year 2011, and conducted research in Case Western Reserve University (US) and The University of Adelaide (Australia). His research focuses on the design and fabrication functional nanomaterials for electrocatalysis. His research accomplishment includes: 1) >210refereed journal articles with a total citation more than 21000 times, 2) 25 invited international conference presentations, 3) 9 research funds as Principal Investigator. He has acted as Advisor board of Nanoscale Horizons (2016-2019), Associate Editor for Materials Reports: Energy (2020-2022), and Advisor board of Materials Reports: Energy (2022-present).

Photoluminescent properties of carbon materials: applications in photovoltaics and MRI Imaging

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Photoluminescent materials are very attractive in solid-state optoelectronic and sensing devices, photovoltaics or medical imaging applications. Recently, various carbon allotropes have demonstrated photoluminescent properties depending on their crystal structure, particle size, surface chemistry and morphology [1]. Although the origin of the photoluminescence emission transition in carbon nanostructures is still unclear, it may be modulated upon the choice of the precursor, the synthetic protocol and the post-functionalization methods [2], opening many possibilities in different application fields. This communication will present an overview of the optical and photoluminescence properties of various carbon materials (e.g., carbon nanostructures, nanoporous carbons) and the dependence of the light emission features on their electronic properties, structural defects and chemical composition. The incorporation of metallic cations -Fe, Co, Mn- into the carbon nanostrustures allows modulating their photoluminescence emission features (broad emission bands between 400-600 nm) and absolute photoluminescence quantum yields between 3-35 %. Although chemical functionalization (heteroatoms) is important, the hybridization of the carbon atoms, the morphology/topology (particle size and aggregation state) and the concentration of the dispersed carbon nanostructures are important parameters that govern the detection of the photoluminescence. Two applications of the prepared photoluminescent carbon materials will be presented: photovoltaics and MRI imaging [3,4]. Mn-containg carbon nanostructures have been tested for in-vitro and in-vivo MRI imaging yielding similar results than commercial gadolinium-based compounds [3]. Unfunctionalized photoemissive carbons have been used as photonic conversion layers in perovskite solar cells, with enchanced efficiency of 1.8% as interlayer of the hole transport material.

Acknowledgements: the financial support of the LEAP-RE program (NANOSOLARCELLS), ECOS-NORD program (CQDs-SOL) and the Romanian Ministry of Research, Innovation and Digitization (PNRR-III-C9-2022-I8-291, contract 760081/23.05.2023) within the National Recovery and Resilience Plan.

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Presenter's Biography

Prof. Conchi O. Ania graduated from Univ. Oviedo (Spain) in 1999 and received her Ph. D in Chemistry in 2003. She performed postdoctoral stays in USA and France. In 2007 she incorporated to Agencia Estatal CSIC (Spain), where she is Research Scientist of Instituto de Ciencia y Tecnología del Carbono (in leave of absence). In 2017 she joined CNRS as Research Director (Orléans, France). She received the national L'Oreal-Unesco 2008 Research Fellowship "For women in Science", for her contributions in advanced technologies based on carbon materials for water remediation. In 2016 she received a Consolidator grant form the European Research Council (ERC) on "Photochemistry based on nanoporous carbons". In 2023 she has received the Silver Medal of CNRS. She is Editor of Carbon journal since 2020. Her research interests focus on nanoporous carbons with tailored surface chemistry and architectures for applications in photocatalysis and electrocatalysis for environmental remediation, gas adsorption/separation, and solar energy conversion (solar fuels, photovoltaics).

2D materials for electronic waste management

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Although highly selective and permeable membranes are sustainable technological solution for clean and low-cost energy, water treatment and healthcare, efficiency and functionality of polymeric and inorganic membranes is still below the dreams of membrane science and technology. For strategical design of novel membranes, we base our technology on the combination of 2D materials and bio-based polymers.

I will talk about our recent works on self-assembly of membranes with catalytic properties and their application for sustainable water treatment and electronic waste management. Designing functional 2D materials and membranes with site-specific functionalities to extract and convert electronic waste offers the potential to imbue active functionality into ion selective membranes. This small-scale tailoring can achieve macro-scale effectiveness, enabling the creation of membranes with intrinsic catalytic properties. Unlike conventional solutions that rely solely on the size sieving properties of membranes our approach combines selectivity and catalysis for the sustainable management of e-waste.

Presenter's Biography

Daria V. Andreeva-Baeumler is an Assoc. Professor in the Institute for Functional Intelligent Materials and Materials Science and Engineering, the National University of Singapore. She is leading a group on programmable membranes with self-adapting and learning capabilities. Daria has authored more than 100 research papers including papers in Nature Nanotechnology, Nature Communication and Advanced Materials and received various fellowships (e.g. Alexander von Humboldt and UNESCO). She leaded a physical chemistry group in the University of Bayreuth, Germany, and worked on smart anticorrosion coatings in Max Planck Institute of Colloids and Interfaces. Having finished her habilitation, she joined the Centre for Soft and Living Matter, South Korea. Daria explores electrochemical phenomena in self-assembled stimuli responsive nanostructures for smart membranes and energy harvesting devices. Of particular interest are semiconductors, piezoelectric crystals and stimuli responsive polymers that operate with ionic currents.

Nanofluidic Energy Storage

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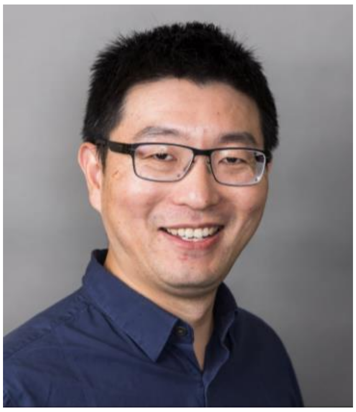
Nanofluidics is the study and application of phenomena that involve fluid (molecule/ion) motion through or past solid nanochannels that measure less than 100 nm in one or more directions. Nanofluidic structures are usually used for power generation through osmotic effects. Recently, ion transport and storage in confinement nanofluidic spaces attract emerging attentions for energy storage research.

In this talk, I would start from pioneering studies on 2D nanofluidic structures (graphene, MXenes, LDH, etc.) in regards of energy storage. Then I would share the thoughts and works from our group in the extension of nanofluidic energy storage through the development of hydrogen-bonded ionic frameworks (HIFs) that have shown encouraging potentials for interesting uses in supercapacitors, batteries and materials derivations. The extension to HIF nanofluidics is a bio-inspired learning journey and hence I would also like to talk about how these new concept materials link energy storage with bio-/eco-friendly technologies. These HIF nanofluidics is developed through a series of mixing H-bondings during spontaneous synthesis processes based on green solvent and self assembly. The selection of the building blocks allows the adjustment of the properties across a fairly reasonable range that is adaptive to different electrochemical environments. Our studies suggest there are more rooms at the centre of the nanofluidic channels for energy storage.

Presenter's Biography

Da-Wei Wang is a Chair Professor at Shenzhen University of Advanced Technology. He was previously a Full Professor and an ARC Future Fellow in the School of Chemical Engineering, UNSW Sydney. His research interest dives into many aspects of sustainable energy, from green materials to system innovations. He is also dedicated to the integration of circular engineering solutions to address sustainable development goals. He has attracted many competitive grants from funding bodies including ARC, CRC, ARENA, and has helped several energy and environment industry partners develop and upgrade new technologies. He has won some awards including the Highly Cited Researcher, Stanford Top 2% scientists, the 2020 Young Scientist Award (under 40) by ICESI, the Finalist of 2018 AMP Tomorrow Maker, and the 2013 Scopus Young Researcher Award by Elsevier & Australasia Research Management Society.



Bio-inspired Nanoionic Materials for Energy Harvesting Devices

Professor Dewei Chu

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Inspired by electric eels, harvesting energy from ubiquitous moisture is attracting growing interest for wearable electronics. Our group have developed a series of carbon nanomaterials based moisture electric generators with superior power output and duration. However, several proposed mechanisms, such as intrinsic gradient of polar functional groups principle and electrokinetic effect perspective, are in wide discrepancy. Here, through the combination of theoretical calculations involving time dimension on material's moisturizing process and experimental analyses, it is revealed the working principle through the water molecule triple roles in driving moisture electric generators (MEGs): 1) intrinsic H_2O absorption on the material surface and splitting into hydroxy group and proton due to the polarizability of the material surface determined by the static electric potential of the materials. This process induces the electrochemical potential difference of the materials via the work function changes; 2) freely diffused protons derived from the H_2O splitting work as the ions charge carriers; 3) via the hydrogen bond of the water molecules to drive charge carriers diffuse between opposite electrodes, maintaining the internal circuit current flow. This work may open a new era of advance for a new energy conversion technology able to directly power wearable electronic devices.

Presenter's Biography: Dewei Chu received his Ph.D. degree in materials science from the Shanghai Institute of Ceramics, Chinese Academy of Science, in July 2008. He worked at the Advanced Institute of Science and Technology (AIST) Japan for three years. He is currently a full professor and ARC Mid-career Industry Fellow in the School of Materials Science and Engineering at UNSW. His research group targets to develop solution-processed, printable, and flexible nanoionic materials for cost-effective and energy-efficient wearable electronics.

Wiring Proton Gradients for Energy Conversion Using Light-Switchable Molecular Switches

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Harnessing light energy for sustainable energy conversion is a key challenge in developing next-generation energy technologies. In this work, we introduce a novel approach using light-activated molecular switches based on merocyanine photoacids to create and control proton gradients in aqueous environments. By carefully manipulating the solvation environment in water-methanol mixtures, these molecular switches can achieve significant changes in acidity, leading to proton concentration gradients of up to 4 pH units under targeted 500 nm light. This controlled light-induced proton transfer process is capable of generating stable open-circuit voltages up to 240 mV.

This research opens new avenues for the design of photo-responsive materials with potential applications in solar energy harvesting. The precise control of proton gradients through molecular switches not only mimics biological energy transduction but also offers a scalable strategy for developing efficient and sustainable energy conversion technologies. Our findings underscore the potential of integrating molecular switches into functional devices, paving the way for advancements in the field of artificial molecular systems and beyond.

Presenter's Biography Dr. Dong Jun (DJ) Kim is a Senior Lecturer and DECRA Fellow at the School of Chemistry, UNSW Sydney. His research focuses on the development of supramolecular materials, with an emphasis on the design and synthesis of novel supramolecular compounds and their detailed characterisation through techniques such as NMR, X-ray crystallography, and electrochemical analysis. These methods are applied to the following main areas: (i) advancing energy storage systems, (ii) developing artificial molecular machines, and (iii) synthetic modelling of key biochemical systems within enzymes.

Scalable Ni-based Electrocatalysts for Hydrogen Electrolyser

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Hydrogen is a highly efficient zero-emission energy carrier, characterized by an energy density of 120 MJ/kg, surpassing that of conventional fuels such as liquefied natural gas (54.4 MJ/kg), coal (27 MJ/kg), and automotive diesel (45.6 MJ/kg).[1] Electrochemical water splitting presents a viable method for producing high-purity green hydrogen, contributing significantly to global decarbonization efforts.[2] The effectiveness of water electrolysis is contingent upon the availability of highly active and cost-effective electrocatalysts. Current electrocatalysts are often constrained by challenging fabrication methods, including high temperatures, hazardous environments, and complex hydrothermal processes, which restrict scalability to an area of m² scale.

In my research, I have developed NiN_x catalysts with rich nitrogen vacancies for the hydrogen evolution reaction, achieving comparable performance to the commercial electrodes through reactive sputtering under room temperature. This method is easily reproducible on various porous substrates and maintains comparable performance to commercial standards.[3] Recently, I also developed NiFeCo catalysts for the oxygen evolution reaction (OER) using a solution-corrosion method. These catalysts demonstrate an ultralow overpotential of 149 mV at 10 mA/cm², are scalable to areas of 10 × 10 cm², and exhibit over 300 hours of operational stability in alkaline electrolyte.[4]

Furthermore, by incorporating trace amounts of iron into the $NiFe(OH)_x$ OER catalysts, I created bifunctional $NiFe(OH)_x$/Fe/graphene catalysts also using the solution-corrosion method, to mitigate ingredient cross-contamination during overall water splitting achieving 10 mA/cm^2 under a cell voltage of 1.51 V.[5]Additionally, I have developed multi-metallic bifunctional catalysts through electrodeposition method, which can be reproducibly fabricated on various substrates with a maximum area of 10 × 10 cm².[6] These fabrication techniques are environmentally friendly and reproducible, holding significant potential for scalable hydrogen electrolyser applications in the future.

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Presenter's Biography

Dr. Doudou Zhang obtained her PhD from Shaanxi Normal University in 2018. During 2018-2019, she spent six months at UNSW as an international exchange PhD student. Subsequently, Zhang began her role as a Research Fellow at ANU in March 2019. She was awarded the Macquarie University Research Fellowships and transitioned to Macquarie University in July 2024. Dr. Zhang, a scientist and mother of two young daughters, focuses her research on solar-driven electrochemical energy conversion, earth-abundant and environmentally friendly low-cost catalysts, and scalable electrolyser technology. She has authored and co-authored 42 publications, including 32 top-tier refereed journal articles, and has an H-index of 16 with over 1,431 citations.

Computational Insight into Ionic Liquids Electrolytes for Lithium and Sodium Metal Batteries

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To meet the ever-increasing demand for high-performance energy storage devices, high-energy-density lithium and sodium metal batteries have become prominent research areas. However, these highly reactive alkali metal anodes are incompatible with the organic solvent electrolytes used in Li-ion batteries due to safety concerns. This presents significant challenges in developing suitable electrolyte materials for practical applications. Ionic liquid electrolytes, consisting of charged cations and anions, have shown promising performance with both lithium and sodium metal anodes. Superconcentrated ionic liquids, which utilize saturated salt concentrations and offer superior cycling stability compared to their low-concentration counterparts, are of great interest. The high salt concentration significantly alters metal ion transport mechanisms and the electrolyte-electrode interface. This presentation provides an overview of our fundamental research into superconcentrated ionic liquid electrolytes through molecular simulations. This includes the understanding of both bulk phase properties and interface behaviour.

Presenter's Biography

Dr. Chen received her Ph.D. in Computational Chemistry from the Centre for Molecular Simulation at Swinburne University in 2012. She is currently working at the Institute for Frontier Materials, Deakin University, leading a Materials Computation and Modelling team, focusing on advancing fundamental research into novel electrolyte materials for applications in high-performance batteries. Her research covers a range of solid and liquid electrolytes, including room-temperature ionic liquids, organic ionic plastic crystals and polyelectrolytes. Using multiscale computational approaches, her research elucidates key mechanisms that control electrolyte properties and performance, providing strategies for the optimal design of novel battery electrolytes, and accelerating future battery development.

Pentagon-rich caged carbon catalyst for the oxygen reduction reaction

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The interaction between electron spin and oxygen molecules in non-platinum catalysts, particularly carbon catalysts, significantly influences the catalytic performance of the oxygen reduction reaction (ORR). A promising approach to developing high-performance catalysts involves introducing five-membered ring structures with spin electrons into graphitic carbons. In this study, we present the successful synthesis of cage-like cubic carbon catalysts enriched with pentagon structures using pentagon ring-containing C_{60} and a NaCl template. The number of pentagons contained in the structure was increased by doping with nitrogen and annealing, and the number of electron spins also increased, thereby improving catalytic activity. The prepared catalyst exhibits remarkable activity in ORR under acidic electrolytes. Furthermore, we elucidate the correlation between the pentagon structure, the number of spin electrons, and catalytic activity, demonstrating that enhanced activity is contingent upon the presence of spin electrons. Density functional theory (DFT) calculations support the role of spin electrons in improving activity. The concept of spin electrons and the introduction of pentagon structures provide new design principles for carbon catalysts.

Presenter's Biography

Guoping Chen received her Ph.D. from the University of Tokyo in 2022. She joined the International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University as a postdoc under the supervision of Prof. Junji Nakamura in 2023. Her current research focuses on self-assembly nanomaterials, fuel cells, and CO_2 conversion applications.

Machine Learning Big Dataset Analysis-Driven C_2 Catalysis

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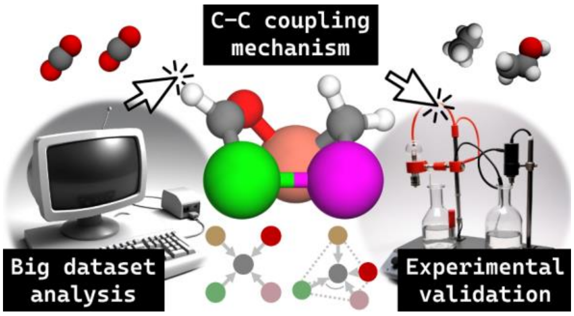
Understanding reaction mechanisms associated with di-carbon species (C_2) is crucial for the electrocatalytic production of green chemicals. However, the optimal direction for potential reaction mechanisms and catalyst material design remains unclear due to the complexity of the reaction network stemming from the intricate chemical structures of C_2. Here, we propose a comprehensive approach to build an extensive dataset encompassing all reactants and catalytic active site compositions to explore reaction mechanisms and screen catalysts through big dataset analysis.[1] Machine learning algorithms developed for various adsorption configurations can quickly and accurately expand quantum chemical calculation data, facilitating rapid access to this extensive dataset. Compared with conventional theoretical methods, big dataset analysis provides a new level of reliability in the results. Importantly, we experimentally confirm the improved performance of CuAgNb catalysts in C-C coupling reactions. We conclude that combining big data with complex catalytic reaction mechanisms and catalyst compositions will establish a new paradigm for accelerating optimal electrocatalyst design.



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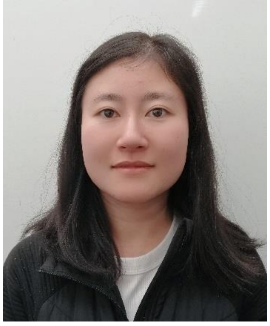
Presenter's Biography



Dr. Haobo Li is an Assistant Professor and independent group leader in Nanyang Technological University (NTU), Singapore. Her research interests center around AI-driven energy chemistry. She received her Ph.D. in 2017 from Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences (CAS). In 2018 she moved to Technical University of Munich (TUM) as an Alexander von Humboldt Postdoctoral Fellow. In 2022, Dr. Li joined The University of Adelaide, where she has been appointed as the sole Chief Investigator for an ARC (Australian Research Council) DECRA (Discovery Early Career Researcher Award) Fellowship. She was awarded the MIT Technology Review Innovators Under 35 (TR35, Asian Pacific) in 2023. She has published over 60 refereed papers (including Science, PNAS, Nature Commun., JACS, Angew., AM, etc.) with a total citation of 9,000 and an h-index of 36 (google scholar).

Carbon Nitride-Based Materials for Light-Assisted Energy and Environmental Applications

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Solar energy utilisation have been greatly driven by the development of photocatalysis, which carries out photocatalytic redox reactions to engage energy and environmental sustainability. Water splitting, oxygen evolution, nitrogen fixation, carbon dioxide conversion, selective oxidation, degradation, and many others have been demonstrated by photocatalysis. The activity, selectivity and stability are determined by the photocatalyst materials. Compared to metal-based semiconductors, the polymeric semiconductor of carbon nitride has become a promising photocatalyst because of the low band gap energy, metal-free nature, easy preparation, and excellent catalytic activity. The surface area and charge separation have restricted its photocatalytic applications. Carbon nanospheres were prepared to attach on the graphitic carbon nitride, and the derived hybrids showed excellent efficiency in photocatalytic degradation of organic pollutants.[1] One-dimensional single walled carbon nanotubes (1D SWCNTs) were used to participate the thermal condensation of melamine, followed by thermal etching to prepared 1D SWCNT/2D C_3N_4. The novel photocatalyst demonstrated efficient activity for overall water splitting.[2] The 2D/2D van der waals heterojunction was achieved by a gas erosion processes on the exfoliated g-C_3N_4.[3,4] Furthermore, C_3N_4/graphene in-plane heterojunction was also designed, and the formation process was investigated in detail.[5] The studies show that metal-free carbon nitride-based hybrid materials can be designed for a variety of applications, such as photocatalytic degradation, selective oxidation, and water splitting, showing great potentials as excellent energy materials.

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Presenter's Biography

Dr. Sun is an ARC Future Fellow and the University Professor of Chemistry in the School of Molecular Sciences at The University of Western Australia (UWA). He previously served as the Professor of Chemical Engineering (Nov. 2017 – Jul. 2023) at Edith Cowan University (ECU). His research focuses on novel catalysis over nanostructured materials for solar-to-chemical/fuel conversion (especially hydrogen) and environmental remediation. He has published over 300 peer-reviewed journal papers, which have received more than 39,000 citations, resulting in an H-index of 107 (Google Scholar). Dr. Sun has been recognised as a Highly Cited Researcher (HiCi) by Clarivate Analytics since 2019 and was named one of the Top 40 Australian Research Superstars by *The Australian* in 2020. In 2023, he was awarded the Mid-Career Scientist of the Year in the WA Premier's Science Awards. Additionally, Dr. Sun serves as a State Government Board Director at the Minerals Research Institute of Western Australia (MRIWA), a member of the ARC College of Experts, and the Editor-in-Chief of Cleaner Chemical Engineering (Elsevier).

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 CO_2 into high value-added carbon products with least energy input, achieving high operational current density under the limited CO_2 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.

Microdesign of Heteroatom-Doped Carbon-Based Energy Storage

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To address the core challenges of low specific energy, poor rate performance, and limited cycling stability in carbon-based energy storage systems, we established a novel in-situ dehalogenation polymerization method for the quantitative synthesis of carbon-based energy storage materials. Various innovative organic and inorganic carbon-based electrode materials with high specific energy and superior stability were designed and developed. These advancements led to the successful demonstration of large-scale energy storage applications with high specific energy, high rate performance, and long cycling life.

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Presenter's Biography

Dr. Huile Jin, male, professor, Ph.D supervisor, he is now the vice dean of College of Chemistry and Materials Engineering, Wenzhou University, Top young talents in Zhejiang Province, Wenzhou high level talents, and the Executive Editor of a Wiley' s journal Carbon Energy. He is vice director of national talent introduction demonstration base, director of Zhejiang Province Key Lab of Leather Engineering, Vice dean of international science and technology cooperation base of micro/nano-structured carbon materials technology.

The design of carbon-based materials with a high mass density and large porosity has always been a challenging goal, since they fulfill the demands of next-generation supercapacitors and other electrochemical devices. His research interest is focused on the design of high-density heteroatom-doped hierarchically porous carbon and metal-free carbon-based electrocatalysts, the study of their fundamentals, and the development of low-cost carbon energy materials and address critical issues in real-world applications. More than 96 patents, over 140 peer-reviewed papers (including ***Nat. Commun., Adv. Mater., JACS, Angew. Chem. Int. Ed., Adv. Energy Mater., Adv. Functional Mater.,*** etc.) with a H index of 31, and 20 invited keynote conference presentations has been contributed. More than 10 patens have been licensed to industry for products development. The one on the production of batteries with multiple rollable cores has significantly reduced the materials and labor cost, which Shenzhen Chenghongyuan Technology Company has benefited for more than 300 million Yuan.

Graphene Oxide: From Preparation to Applications

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Graphene has excellent properties, such as high mechanical strength and modulus, high thermal and electrical conductivities, very good thermal and chemical stabilities, and unique electronic properties. So graphene is expected to be used in various applications. Graphene oxide is one of the most versatile graphene materials which has been widely investigated and used. We have developed a free radical oxidation method to produce graphene oxide in large quantity with low pollution, and then a centrifugal fluid alignment process to assemble graphene oxide membrances with different thicknesses which can be converted into graphene membranes with a high thermal conductivity. These graphene membranes have been used in electronics and optoelectronics for efficient thermal management. Interestingly, we have found that partially-reduced graphene oxide has a high gold extraction capacity from electronic waste (e-waste), one order of magnitude higher than other reported gold adsorbents. During extraction, the reduced graphene oxide reduces >95% gold ions to metallic gold, avoiding elution and precipitation necessary in post-adsorption processing. Moreover, this reductive adsorption of gold by reduced graphene oxide is found different from (predominately) electrostatic adsorption of other metal ions, hence, having precise gold extraction without adsorption of other 14 elements present in e-waste. Most recently we found that graphene nanosheets can be “sintered” into strong bulk graphite materials at a mild temperature of 45 degree C. However, great efforts are still needed for the research, development, and commercialization of graphene oxide and their deriatives.

Presenter’s Biography

Prof. Hui-Ming Cheng is the founding director of the Institute of Technology for Carbon Neutrality, Shenzhen Institute of Advanced Technology, CAS, and the honorary dean of Faculty of Materials Science and Energy Engineering, Shenzhen University of Advanced Technology. He is concurrently the director of the Advanced Carbon Research Division of Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS. He is a member of CAS and a fellow of TWAS. His research activities mainly focus on energy materials and devices, carbon nanotubes, graphene, and other 2D materials. He has published over 900 papers with an h-index of 166, and is a Highly Cited Researcher in three fields of materials science, chemistry, and environment and ecology. He has given over 220 plenary/keynote/invited lectures at various conferences, and won quite many domestic and international awards. He is now the founding Editor-in-Chief of Energy Storage Materials and has spun off several high-tech companies.

Catalytic mechanisms for ROS generation from metal-free carbon catalysts

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ROS-induced cell death could be one of the attractive options for cancer therapy.[1] The development of targeted nanomaterials offers a promising strategy for cancer therapy by enhancing selectivity and reducing side effects.[2] In this study, we synthesized a metal-free, targeted carbon nanomaterial that selectively recognizes cancer cells and induces apoptosis through the efficient generation of reactive oxygen species (ROS), leading to oxidative stress and activation of apoptotic pathways. By conjugating folic acid (FA) to receptor proteins on the cancer cell membrane, the specifically FA-defected carbon nanotubes (FA-RN-CNTs) target cancer cells and nitrogen removed defects efficiently catalyze ROS generation. Cell viability assays confirmed that the targeted FA-RN-CNTs nanomaterials exhibit significant cytotoxicity (IC_{50}=9.065 μg/ml) toward MDA-MB-231 cancer cells while sparing NIH-3T3 normal cells among purified CNTs, nitrogen doped CNTs and defected CNTs. The selective induction of apoptosis via ROS generation and the subsequent activation of specific apoptotic pathways highlight the potential of this nanomaterial as a therapeutic agent. This process results in the upregulation of pro-apoptotic proteins such as BAD and downregulation of anti-apoptotic proteins such as Bcl-2, triggering intrinsic mitochondrial apoptosis in cancer cells and producing significant anticancer efficacy. This is the first demonstration that specifically FA-RN-CNTs can catalyze ROS generation within the tumor microenvironment, and we have elucidated the associated catalytic mechanisms. This work opens new avenues for the development of safe and efficient targeted catalytic nanomedicines for effective cancer treatment.

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Presenter's Biography

Huiqian Qi is a Ph.D. candidate in the Department of Chemcial Engineering at the University of New South Wales. She received full scholarship funded by UNSW-University International Postgraduate Award (UIPA). She received her MS Materials Science and Engineering degree from University of New South Wales in 2021. Her research interests focus on the synthesis and applications of advanced carbon-based materials for biosensors, biomedical and energy related applications. She has published three research papers, including one first-authored article, and one Chinese Invention Patent (Individual, Application Granted).

Design and Optimization of a Black Plasmonic-Au Paper Based Solar Water-Evaporation System with Enhanced Efficiency and Stability

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Interfacial solar water evaporation (SWE) is a promising technology that addresses the challenge of providing fresh water in water-scarce regions. Among the various factors affecting performance, effective heat-loss management and precise control of the water feed rate are crucial for maximizing steam generation efficiency. In this study, we present the design of an SWE system based on a single black plasmonic-Au paper (BPAP), engineered to minimize conductive heat loss and optimize the water feed rate. The efficiency of the system was evaluated using two approaches: (i) based on the latent heat of vaporization and (ii) by accounting for all potential heat losses.

Our findings reveal that conductive heat loss to the bulk liquid can result in an 18% reduction in efficiency, impacting the steam generation rate. Here, the water feed channels were carefully designed to sustain evaporation rates of > 2.0 $kg·m^{-2}·h^{-1}$, with only 2% of the incident energy lost due to conduction to the cold water. The developed system demonstrates excellent performance and stability, achieving evaporation rates ranging from 1.5 to 2.1 $kg·m^{-2}·h^{-1}$ under 1-sun illumination. Furthermore, the system maintained consistent performance over 168 hours of continuous operation without any detectable material properties or efficiency degradation. This work offers valuable insights into the design of high-efficiency SWE systems and presents a viable solution for freshwater production in water-scarce regions.

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Presenter's Biography

	Ilsun Yoon is an Associate Professor in the department of chemistry at Chungnam National University (CNU), Korea. He received BS/MS/PhD degrees in chemistry from KAIST. He worked as a postdoc researcher at KAIST, University of California San Diego, and a principal research staff at Samsung Advanced Institute of Technology. He joined CNU as an Assistant Professor in 2014. His research is focused on advanced optical and photonic materials for sensors and energy devices, including SERS, LED, photovoltaics, and solar desalination.

Chiral catalyst effect of twisted nanowire bundles for photoelectrochemical water splitting

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The overexploitation of fossil fuels has made developing alternative energy sources essential. Photoelectrochemical (PEC) water splitting is a promising method for hydrogen generation, considered the fuel of the future due to its high enthalpy of combustion. However, PEC water splitting efficiency is still insufficient for large-scale hydrogen production, requiring further efforts. Recently, chirality has been shown to play a crucial role in addressing PEC water splitting issues through chiral-induced spin control and enhanced light harvesting. Focus on chirality is now critical to improve water splitting efficiency. This research outlines methods for integrating achiral structures into photocatalysts for PEC water splitting. The current study proposes an innovative approach to induce achiral structures that exhibit circular dichroism under chiral experimental conditions. Specifically, twisted nanowire bundles introduce a chiral effect, improving light absorption essential for generating electron-hole pairs in PEC systems. We present advanced results demonstrating the chiral catalyst effect of twisted nanowire bundles. The unique CoO3-CuMoS2 nanostructures enhanced photoanode interface charge transfer to 10.68 mAcm^-2 at 1.23 V RHE. Additionally, computational modeling substantiates the catalytic properties and helps identify the optimal geometric configuration of nanowires. COMSOL Multiphysics simulations were conducted to examine the material's optical properties. The paper discusses the challenges of activating PEC water splitting and anticipates a promising future for this technology. In summary, while PEC water splitting holds significant potential for hydrogen production, achieving efficiency requires innovative approaches. Introducing chiral effects via unique nanostructures, such as twisted nanowire bundles, represents a significant advancement. The combination of experimental results and computational modeling provides a comprehensive understanding of the mechanisms involved, paving the way for future developments in this field.

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Presenter's Biography

Recent Photo 
Name (Affiliation): Prof. Jaebeom Lee(Chungnam National University, Korea)
Presentation Title: Chiral assembly of magnetoplasmonic nanohybrid materials for THz metasurface

Prof. Jaebeom Lee has been engaged in research on nanoparticle and nanostructure synthesis, biosensors, and energy catalysis for more than 17 years and has published +260 papers in high-impact factor journals such as Science, Nature Materials, Science Advances, JACS, Angewantde Chemie, Nano Letters, ACS Nano, Advanced Functional Materials, Advanced Optical Materials, Nano Today, ACS Photonics, and other high-impact factor journals, including +80 patents, 8 technology transfers (worth 800 million won, +50 million won in royalties), and 2 startups, and mass-produced 10 commercialized products. So far, Graduated 10 postdocs, 20 PhDs (12 professors), and 10 master's students. Currently operating a laboratory with 12 researchers (2 research professors, 8 PhDs, and 2 MSc students). Received the 2011 Pusan National University Best Research Award, 2014 Nano Korea Top 40 Inventions of the Year Award, 2017 Prime Minister's Award for Education, and 2023 Youngin Outstanding Academic Research Award and 2024 Chungnam National University Best Research Award.

Defect-engineered nanomaterials as in situ quantum sensors

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Wide bandgap semiconductors such as diamond and hexagonal boron nitride (hBN) are known to host point defects that harbour an optically addressable electronic spin. These systems can be used as quantum sensors, able to detect tiny magnetic signals for instance from nearby paramagnetic molecules. In this talk, I will present our work on the engineering and applications of such quantum sensors. First, I will talk about sensing and imaging with nitrogen-vacancy centres in diamond, and present applications in materials characterisation, chemical sensing, and temperature monitoring [1-3]. In the second part, I will talk about a class of defects we discovered in hBN nanomaterials and the opportunities they open for sensing [4-6].

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Presenter's Biography

Jean-Philippe Tetienne is an ARC Future Fellow and leader of the Quantum Sensing group at RMIT University. He received his PhD in 2014 from ENS Cachan, France, and worked as a Research Fellow and ARC DECRA Fellow at the University of Melbourne from 2015-2020, prior to joining RMIT in 2021. His research group specialises in the physics and engineering of optically addressable spin defects in solids, particularly diamond and hexagonal boron nitride. His group also develops quantum sensing technologies based on those systems, including precision magnetic microscopes for materials science and geological exploration, and high-sensitivity magnetometers and RF receivers for defence and space applications.

Sustainable synthesis of carbon materials using molten salt electrolysis

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Sustainable processing solutions require technologies that not only run on renewable electricity, but that also consider the complete supply chain of materials involved to ensure overall outcomes are better than business as usual. Manufacturing has traditionally depended on the use of fossil fuels, not just for electricity but as chemical feedstocks to generate materials at scale. Future solutions must be completely decarbonised including component manufacture.

Here, the generation of advanced carbon materials using molten salt electrolysis technology will be discussed for energy and other applications. Carbonate salts enable fast and efficient transformation of carbon dioxide gas into a variety of advanced carbon materials [1]. From modification of carbon structure (graphitic/amorphous/hard carbon [2], recent evidence of diamond deposition [3]), through to doped carbon materials (silicon and iron [4] doped carbons), the flexible electrolytic process method discussed produces tuneable carbon materials with an overall carbon negative emission footprint.

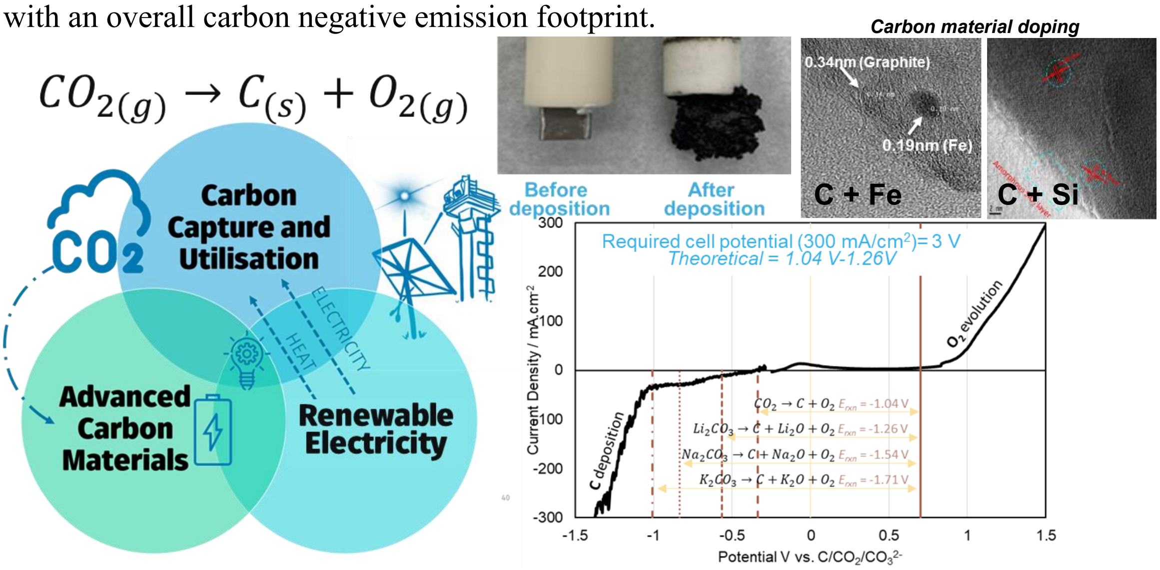

Figure: (LEFT) Complete reduction of carbon dioxide to advanced carbon materials, (TOP RIGHT) cathode before and after carbon deposition, doped iron [4] and silicon materials TEM, (TOP LEFT) electrochemical response in carbonate salts at an iron electrode [1].

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Presenter's Biography

Dr Jessica Allen is currently leading the Electrochemical Engineering Laboratory at the University of Newcastle with the Newcastle Institute for Energy and Resources. Dr Allen is a Senior Lecturer in chemical engineering and is a 2021 Australian Research Council DECRA fellow. Dr Allen has a multidisciplinary background spanning chemistry and engineering and has spent time in industry as a professional engineer. She is passionate about technology development and science communication and believes both are critical in the fight against catastrophic climate change.

Strategies for hydrogen production

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Hydrogen is considered the cleanest energy and has been the focus of research recently. In the last three years, we have used different strategies for improving hydrogen generation, including doping, heterostructure, synthesizing new materials and external excitation. In addition, electrochemical catalytic reaction, photocatalytic reaction and electro-photocatalytic reaction methods have been employed for hydrogen production. With these strategies and different catalytic reaction techniques, the hydrogen production rate is strongly enhanced.

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Presenter's Biography

Jiabao Yi is a professor of the Global Innovative Center of Advanced Nanomaterials, The University of Newcastle (UON). His research intersts focus on advanced functional materials including magnetic semiconductors, magnetic nanoparticles, oxides, 2D materials and their applications in energy storage and conversion. He obtained Lee Kuan Yew postdoc fellowship in Singapore, QEII and Future Fellowship in Australia.

An interface-enhanced continuous 2D-carbon network enabling high-performance Si anodes for Li-ion batteries

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Silicon (Si) has been regarded as a promising anode material for next-generation Li-ion batteries by virtue of its high theoretical capacity and low working potential. Although various strategies have been proposed to solve the problems of Si anodes (e.g., poor electrical conductivity and volume effects), there is still a lack of efficient ways to simultaneously realize the high capacity, good rate capability and stability of Si anodes. Herein, an interface-enhanced 2-D carbon network is introduced into the Si anode by a simple templating method using gelatin as a carbon precursor. Electrochemical measurement, in situ Raman spectroscopy, and theoretical simulation results suggest that the unique gelatin-derived carbon nanosheet (GCNS) structure not only promotes the Li-ion diffusion and electron transport within the Si anode, but also stabilizes the Si structure. The Si anode having the interface-enhanced GCNS network (Si@GCNS) exhibits high charge capacity (2975 mA h g^{-1} at 0.2 A g^{-1}), good rate capability (1892 mA h g^{-1} at 5 A g^{-1}), and long lifetime (with a capacity retention of 83.4% after 400 cycles), superior to the Si-based anodes modified by 3-D or 2-D carbons. Moreover, a pouch cell based on the Si@GCNS anode and a commercial $LiFePO_4$ cathode shows a high energy density of ∼460 Wh kg^{-1} and good cycling performance.

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Graphatic materials for energy applications

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I will introduce several types of graphitic materials [1-4] with high conductivity and high light absorption fabricated from bulk scalable carbon materials. I will discuss the application of high conductivity as an energy storage material, and explain how the advantage of high absorbance is utilized in solar desalination as a photoabsorber. High conductivity and large surface area are critical properties for active materials in energy storage devices including supercapacitors and batteries. The 3D graphene developed by our group meets both of these conditions exceptionally well and therefore showed good performances as energy devices. Solar desalination is a promising way to produce fresh water utilizing the solar energy. We designed a circular type 3D-supporter whose top surface was concave using 3D-priting, which allowed for effective light harvesting. The solar energy was absorbed multiple times and improved the capability of light harvesting of highly absorptive graphitic materials. Based on these designs, we obtained a relatively high evaporation efficiency of 89%.

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Presenter's Biography

Ji-Hyun Jang is a professor of the school of Energy and Chemical Engineering at Ulsan National Institute of Science and Technology (UNIST) in Korea. She received Ph.D. degree in chemistry from Korea Advanced Institute of Science and Technology (KAIST), Korea, in 2004. Then, she conducted postdoctoral research in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology (MIT) sociate, working on the fabrication of 3D nanostructures via interference lithography. Since 2009, she has been with the School of Green Energy, at UNIST. Her research has been focusing on new nanomaterials and understanding their functions in energy processes, including photocatalysis for hydrogen generation and electrochemistry for energy-storage devices. She is also deeply involved in synthesizing and developing physicochemical properties of the wonder 2D materials. She is currently an Associate Editor of of *Materials Today Energy*.

Improving the Thermal Stability and Oxidation Resistance of High Temperature Carbon Fibre Composites

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This work studies the effects of nanofillers on improving the thermal stability and oxidation resistance of carbon fibre reinforced high temperature phenolic resin composites. For the low viscosity phenolic resin composites investigated, it was found that high-quality, low-porosity carbon fibre reinforced composites can be fabricated through vacuum-assisted resin infusion. Incorporating ZrO_2 nanoparticles into the phenolic resin significantly enhances the thermal stability of carbon fibre phenolic composites, as well as their residual strength and stiffness after prolonged exposure to elevated temperatures. Composites with 1 wt% ZrO_2 nanoparticles exhibited a substantial improvement in residual strength and stiffness—65.4% and 48%, respectively—compared to unmodified composites after a 30-second heat exposure in a cone calorimeter at a heat flux density of 90 kW/m². This enhancement in thermal stability is attributed to the improved chain stability of the phenolic polymer, the thermal absorption properties of ZrO_2, and the catalytic behavior of ZrO_2, which increases carbon yield within the composites.

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Presenter's Biography

J*in Zhang* is a Scientia Associate Professor and an Australian Research Council Future Fellow at UNSW Sydney. Her current research interests cover functional nanocomposites for energy harvesting and sensing, lightweight structural fibre reinforced polymer composites for photovoltaic modules and cryogenic storage tanks, biodegradable composites for packaging, etc. She received Endeavour Fellowship from the Department of Industry, Innovation, Science, Research and Tertiary Education, Australia in 2012 and Victoria Fellowship from the Department of Victorian State Development Business and Innovation in 2013. She is leading multiple research projects for sustainable materials, energy, and technologies.

Carbon structure, chemical bonding, and reaction processes probed by soft X-ray spectroscopy

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Carbon is a remarkable element showing a variety of stable forms ranging from 3D semiconducting diamond to 2D semimetallic graphite to 1D conducting and semiconducting nanotubes to 0D fullerenes. Carbon-based materials (clusters, molecules and polymers), which show many interesting properties, are unique in many ways. The unique ability of carbon atoms to form single, double, and triple covalent bonds through different types of hybridization effects considerable variability in the structure and physical properties. This accounts for the variety of known allotropes, permitting industrial and technological applications ranging from industrial lubricants and batteries to moderators in nuclear reactors.

I have performed soft X-ray spectroscopy experimental study on a variety of carbon systems (diamond, graphite, fullerenes, conjugated polymers, graphene) which have yielded characteristic fingerprints. Soft X-ray absorption spectroscopy (sXAS) and resonant inelastic X-ray scattering (RIXS) are element specific techniques that have been used to investigate the electronic and structural changes in the battery electrode materials. Depending on the detection method, sXAS can be either surface sensitive (detection depth of ~5 nm) or bulk sensitive (detection depth of ~100 nm), which enables XAS as a probe of distinguishing the surface and bulk reactions in battery electrode materials, such as reduced graphene oxide, and B-/N-doped graphene oxides, and also in catalytic reactions, for example, the interfacial layer facilitating photogenerated electron transfer from the SiC substrate to the graphene active sites, affording efficient CO_2 activation and C-C coupling to produce C_2H_5OH.

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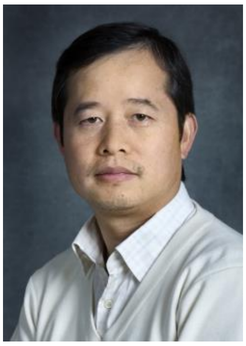
Presenter's Biography



Jinghua Guo is a Senior Scientist, Lead of RIXS Program of Photon Science Group at the Advanced Light source, Lawrence Berkeley National Laboratory, adjunct professor in the Department of Chemistry and Biochemistry, University of California, Santa Cruz. He received his PhD in Uppsala University, Sweden in 1995, M.S. in Shanghai Institute of Optics and Fine Mechanics, Chinese Science Academy, China in 1988, B.S. in Zhejiang University, China in 1985, and joined Lawrence Berkeley National Laboratory in 2001. His research focuses on soft X-ray spectroscopy of nanostructured materials, energy storage materials, catalysis, and chemical processes. He has developed novel instrumentation of in-situ/operando soft X-ray spectroscopy for studying energy materials, electrochemical and catalytic reactions in the real-world conditions. He has published over 510 peer-reviewed articles with Google Scholar Citations over 39350 and h-index of 99.

Atomic-Level Regulation on Photocatalyst for Energy-Related Reaction

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The global energy crisis and environmental issues impel the aggressive search for a clean and renewable energy source to replace fossil fuels. Hence, conversion of renewable solar energy into clean fuels and valuable chemicals is of great significance. The core challenge of this advanced technology lies in the development of low-cost and environmentally benign photocatalysts with sufficiently high activity and stability. Hence, the rational design and synthesis of photocatalysts at the atomic level to achieve efficient and stable solar-to-chemicals conversion is highly promising. Furthermore, both advanced characterizations (e.g., aberration-corrected atomic-resolution transmission electron microscopy, synchrotron-based X-ray absorption spectroscopy and various in-situ element/space/time-resolved characterizations) and density functional theory based theoretical computations are adopted to investigate the atomic-level structure/composition-performance relationship and mechanism in photocatalysts. Finally, a universal rule to develop high-performance photocatalysts for efficient solar-to-chemicals energy conversion is concluded.

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Presenter's Biography

Dr. Jingrun Ran is appointed as a senior lecturer and ARC future fellow in school of chemical engineering in University of Adelaide. He was awarded with the ARC DECRA fellowship in 2020. His research is focused on the atomic-level regulation on photocatalysts for producing energy fuel and value-added chemical using renewable solar energy. He has been recognized as a Clarivate Highly Cited Researcher in 2020-2024, and recognized as the world's top 2% scientists (released by Stanford University) in 2020-2023. He has also been recognised as a Journal of Materials Chemistry A Emerging Investigator in 2021. He has published 65 papers in well-renowned journal, including Nat. Commun., Adv. Mater., Angew. Chem. Int. Ed., Energy Environ. Sci., J. Am. Chem. Soc., Adv. Energy Mater., Chem. Soc. Rev., Sci. Adv. (over 19259 citations, h-index: 42 based on google scholar).

Refining structures of electrochemical catalysts for energy storage and conversion

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The development of highly efficient catalysts to improve the electrochemical performances is urgently needed due to the ever-increasing demand for energy storage and conversion devices in the last few decades. However, the electrochemical performances are still not satisfying to be potentially used in industrial applications. Here, we present our recent research on the structure tuning for electrocatalysts designed for energy storage and conversion devices such as Li-O_2 batteries and electrochemical water splitting.[1-5] We show that by carefully designing and tailoring the molecular and electronic structures, the efficiency of the applied catalysts could be maximized which would be highly beneficial for the electrochemical performances in their individual applications. For instance, TEMPO-modified ionic liquid could stabilize the lithium anode and prolong the cycle life of Li-O_2 battery,[2] while in-situ exfoliated MXene coupled with single Pt atoms show a mass activity more than 40 times higher than the commercial Pt/C.[4] All these provide theoretical and experimental guidance to develop highly efficient catalysts for energy storage and conversion devices in the future.

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Presenter's Biography

Jinqiang Zhang obtained his PhD degree from the University of Technology Sydney in 2018. He has worked as a Postdoctoral Research Associate in the Centre for Clean Energy Technology at the University of Technology Sydney from 2018 to 2021, and a Postdoc Research Fellow at the University of Toronto from 2021 to 2023. He is currently a Chancellor's Research Fellow and DECRA Fellow at the University of Technology Sydney. His work mainly focuses on the design and synthesis of functional organic molecules and single-atom catalysts in energy conversion and storage systems such as hydrogen evolution reactions, oxygen evolution reactions, oxygen reduction reactions, CO_2 reactive capture, lithium-ion batteries, lithium–sulfur batteries, and lithium–air batteries.

Atomically Dispersed Electrocatalysts for Low Temperature Fuel Cells, Water Electrolysis and Li-S battery

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Single-atom catalysts (SACs) have attracted growing attention because the number of active sites, with unpredictable catalytic activity can be maximized. Despite numerous studies on SACs, there is little research on the support, which is essential to understanding SAC. In this presentation, we report on the influence of the support on the performance of the SAC by comparing with single-atom Pt supported on carbon (Pt SA/C) and Pt nanoparticles supported on WO_{3-x} (Pt NP/WO_{3-x}). The results revealed that the support effect was maximized for atomically dispersed Pt supported on WO_{3-x} (Pt SA/WO_{3-x}). The Pt SA/WO_{3-x} exhibited a higher degree of hydrogen spillover from Pt atoms to WO_{3-x} at the interface, compared with Pt NP/WO_{3-x}, which drastically enhanced Pt mass activity for hydrogen evolution (up to 10 times). This strategy provides a new framework for enhancing catalytic activity for HER, by reducing noble metal usage in the field of SACs. We have designed an oxophilic support material, WC_{1-x}, for SAC to enhance the HOR activity of Ru SAC in alkaline condition by lowering the PZC of the electrode sufficiently to adsorb negatively charged OH^- even in the HOR potential region. We also prepared Fe-N-C catalysts with tunable catalytic activity for oxygen reduction reaction (ORR). The binding energy of oxygen intermediate was controlled by changing the functional group around Fe-N-C catalysts.

Presenter's Biography

Prof. LEE is currently a Chair Professor at KAIST, Daejeon, Korea. His research field of interest is nanostructured electrocatalysts for water electrolysis, fuel cells and Li-S batteries.

He started his professional career as an Assistant Professor in Department of Chemical Engineering at POSTECH (2008-2018), and moved to KAIST in 2018 where he was later appointed as the KAIST Chair Professor.

He has published more than 270 papers including Nature Materials, Nature Catalysis, Nature Comm. JACS, Angew. Chem. Energy. Env. Sci., Adv. Mater., and ACS nano. Total citation number and H-index are 29045 and 90, respectively. He has served as an Editor for Chemical Engineering Journal (Elsevier, Impact factor 13.3-Novel Materials for Energy Section) since 2017.

He received the B.S. degree from the School of Chemical and Biological Engineering at Seoul National University, Korea in 1993. He then received the Ph.D. degree from the School of Chemical and Biological Engineering at Seoul National University, Korea in 1998. After postdoctoral research at SNU (with Prof. Taeghwan Hyeon) and Cornell University (with Prof. Ulrich Wiesner), he joined the faculty of the Department of Chemical Engineering at POSTECH (2008–2018)

Data-driven Design of Carbon-based Single-atom Catalysts for Electrochemical Ammonia Synthesis from Nitrate

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With high atomic utilization and excellent stability, carbon-based single-atom catalysts have shown promising performance in the electrochemical synthesis of ammonia from nitrate. To achieve efficient catalyst development and design, we introduced a data-driven approach based on density functional theory (DFT), bypassing traditional time-consuming trial-and-error methods. Here, we propose various catalysts featuring single metal atom sites embedded in nitrogen- and oxygen-co-doped porous carbon (M-NO/C), identified through high-throughput computations. Theoretical calculations reveal that the NO3RR activity of M-NO/C originates primarily from optimized charge transfer between uniformly distributed metal and oxygen atoms. This configuration significantly accelerates water dissociation for proton supply and effectively reduces the Gibbs free energy of the rate-determining step (*NO → *NHO). Guided by these calculations, we successfully developed a Cu single-atom catalyst exhibiting high ammonia Faradaic efficiency and yield at low potential, outperforming most existing metal-nitrogen carbon single-atom catalysts.

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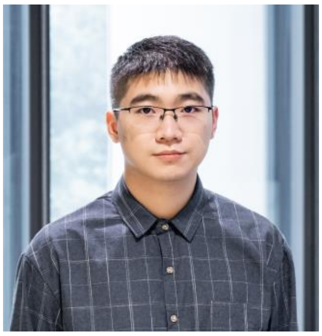

Jinyang Guo is a Ph.D. candidate in the group of Prof. Liming Dai and Prof. Zhenhai Xia in the School of Chemical Engineering at the University of New South Wales. His current research interests focus on earth-abundant catalysts design for energy conversion and green chemistry (metal-air batteries, water splitting, electrochemical urea synthesis, etc.). His research involves multiscale modeling, DFT simulation, mechanism study, and catalytic activity prediction.

Exploring the potential of stipa tenacissima and other biomass resources for hard carbon production in na-ion batteries

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High-energy sodium-ion batteries (SIBs) are emerging as advanced alternatives to lithium-ion batteries due to sodium's abundance and diverse compounds. Biomass-derived hard carbon, known for its cost-effectiveness and customizable properties, shows great potential to enhance sodium storage capacity and performance. This talk highlights the use of Stipa tenacissima (ALFA plant), a resilient North African biomass, as a sustainable source for producing high-performance carbon materials for SIBs, showcasing how abundant biomass resources can drive progress in energy storage.

Conventional hard carbons are typically produced from synthetic organics and lignocellulosic biomass. However, the environmental and economic downsides of synthetic organics—such as increased CO2 emissions and reliance on costly petroleum resources—emphasize the need for more sustainable options. Lignocellulosic biomass, including perennial plants and agricultural by-products, presents a renewable, eco-friendly alternative with notable economic benefits.

Our research investigates hard carbons derived from Stipa tenacissima for sodium-ion batteries (SIBs). The structural properties of ALFA plant-derived hard carbons—such as their disordered structure, low graphitization, larger pores, and widely spaced graphene sheets—make them highly effective anode materials. These features offer abundant active sites for sodium ion intercalation and deintercalation, resulting in improved battery performance.

In addition to Stipa tenacissima, this presentation will explore the potential of various biomass resources for hard carbon production. A central focus will be the impact of different pyrolysis conditions on the structural and electrochemical properties of these materials, highlighting the importance of optimizing these parameters to achieve high-energy densities and enhanced reversible capacities in SIBs. Additionally, advanced techniques such as heteroatom doping, activation modification, and chemical cross-linking, will be investigated as strategies to enhance the carbonization process, increase material yield, and improve overall electrochemical performance, paving the way for advancements in SIBs technology.

Jones Alami, is Professor, holder of the sustainable energy chair, and head of the MSN Department at UM6P in Morocco. He is the co-founder and CEO of NGB Materials, an LFP company since December 2023. Jones has a Doctorate in plasma physics (2003) and a PhD in thin film physics (2005) from the University of Linkoping in Sweden. After post-doctoral studies at Aachen University in Germany, he joined industry as a Research Manager and Innovations Manager, before founding INI Coating, a coatings R&D company, and simultaneously occupying the position of Joint Professor for three years at the prestigious SICCAC in China. Dr. Alami has more than 150 peer-reviewed publications and is the author/co-author of over 30 patents and patent applications.

Mechanochemistry for materials synthesis

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Conventional reactions are mostly driven by heat, light, and electricity. They are named as thermochemistry, photochemistry, and electrochemistry, respectively. Likewise, chemical reaction, caused by mechanical actions, is defined as mechanochemistry, which delivers energies required to overcome reaction barriers via abrasion, friction, cracking, colliding, and so on. The most representative tool for operating mechanochemistry is ball-milling, which can offer a new avenue for sustainable materials synthesis, including (1) single atom catalysts (SACs) from bulk metal balls, (2) methane from char coals, and (3) ammonia from nitrogen. Various SACs can be produced by a top-down mechanochemical abrasion method, in which the bulk metal balls (single atom percussors) are directly atomized onto different substrates, such as carbon frameworks, oxides, carbides, and nitrides.[1] Carbon frameworks, such as char coals in the presence of hydrogen (carbon hydrogasification), can also be efficiently converted into methane via mechanochemical ball-milling.[2] The rate of carbon hydrogasification is four orders of magnitude higher than the conventional thermochemical method. Furthermore, ammonia has mainly been produced by the Haber-Bosch process over 110 years. However, it cannot be performed under mild conditions, because of thermodynamic reasons. We have discovered a new method for the synthesis of the ammonia under mild conditions (45 °C and 1 bar) via mechanochemical ball-milling iron (Fe) catalyst in the presence of nitrogen and hydrogen.[3] With this new process with potassium (K) promoter, the final concentration of ammonia have reached as high as 94.5 vol%,[4] which is nearly 4 times higher than the state-of-art Haber-Bosch process (~25 vol%) under harsh conditions (450 °C and 200 bar). Stable nitrogen dissociation at the mild conditions is associated with mechanochemically induced high defect density and violent mechanical actions on the Fe catalyst.[5]

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Jong-Beom Baek's Biography

Jong-Beom Baek is a distinguished professor/director of the Department of Energy and Chemical Engineering/Center for Dimension-Controllable Organic Frameworks, Ulsan National Institute of Science and Technology (UNIST), South Korea. Currently, his research interests include the syntheses of two- and three-dimensional high-performance organic network structures and the chemical modifications of carbon-based materials for multifunctional applications, including energy conversion and storage.

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.[5] 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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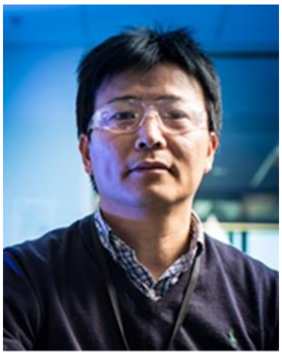
5. Q. Wu, etc al., *Nature Communications*, 2023, 14, 6275.

Biography

Professor Jun Chen is currently appointed as Deputy Director 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).



Advanced Design of Vanadium-Based Cathode Materials for High-Performance Aqueous Zinc-Ion Batteries

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Vanadium-based aqueous zinc-ion batteries (V-ZIBs) have garnered significant attention in the field of electrochemical energy storage due to their potential for high-performance applications. This report focuses on the design of vanadium-based cathode materials, employing strategies such as doping and functional interface engineering to regulate the intercalation ratio of protons and zinc ions. By introducing different doping elements, the electronic conductivity and structural stability of the cathode material can be significantly improved, enhancing the high-rate performance of the battery. Additionally, functionalized interfaces help reduce interfacial resistance, further boosting charge transfer efficiency. The controlled co-intercalation of protons and zinc ions enables large capacity charge storage and release. In terms of cycling stability, these tuning strategies greatly enhance the structural robustness and durability of the cathode material, allowing vanadium-based ZIBs to maintain excellent electrochemical performance over extended cycling.

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Presenter's Biography

Dr. Jun Li is a Distinguished Professor at Wenzhou University. He was awarded the National Scholarship for Doctoral Studies at University of Windsor, Canada. After graduation, he went back to China and worked at Sichuan University for two years. He also served as a visiting scholar at the University of Windsor, Canada. Dr. Li has long been dedicated to the research of synthesizing nanomaterials through the regulation of chemical reaction kinetics, with a focus on energy storage and conversion applications. Over the past five years, he has led two National Natural Science Foundation projects and published over 80 SCI-indexed academic papers in prestigious journals such as ***Adv. Mater., Angew. Chem. Int. Ed., Adv. Energy Mater., Nano Energy, Energy Storage Mater.*** Several of his research outcomes have been featured by scientific media outlets both in China and internationally. He has been invited to deliver reports at numerous international and domestic conferences and universities and holds over 20 authorized Chinese invention patents.

Efficient ion separation by metal-organic framework membranes

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Ion separation by nanoporous membranes has become a research hot spot in the fields of nanofluidics and membrane separation because of its wide potential applications, such as lithium extraction, osmotic energy harvesting, and ion sensing. Biological ion channels, featuring outstanding single-ion selectivity, set a high bar for ion selectivity and the gradual understanding of the structure-property relationship of biological ion channels has inspired scientists to design and fabricate diverse nanoscale and subnanoscale platforms to achieve desirable ion selectivity. In this aspect, the advent of nanofabrication and emerging carbon-based porous materials with nano-channels or subnanochannels enable researchers to construct various nanoconfined spaces to investigate the ion selectivity. It is fundamentally important to achieve atomic-scale selective ion transport by artificial membranes to gain an deep insight into the principle of selective ion transport under nanoconfinement. In addition, tuning the macroscopic structure of membranes, such as asymmetric or heterogeneous structures in terms of both aperture size and charge density can impart multiple-functional ion separation comparable to cell membranes. Metal−organic frameworks (MOFs) are a promising class of crystalline porous materials with desirable structures for constructing controllable nanometer platforms as an alternative to other carbon materials, such as polymers and two dimensional (2D) layered materials for fabrication nanometer plaforms to investigate the selective ion transport. As on of the earliest groups engaged in ion separation, we have constructed a series of unprecedented MOF-based sub-nanochannel membranes to achieve pioneering ion selectivity comparable to biological ion channels: 1) acidic MOF membrane to achieve rectifying monovalent/divalent metal ion selectivity[1]. 2) MOF-macrocyclic sub-nanochannel membrane to achieve ultrahigh Na^+/K^+ selectivity[2].

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Presenter's Biography

Jun Lu received his Master degree from Tianjin University in 2013 and Ph.D. degree from Monash University in 2020 and currently works as an ARC DECRA fellow at Monash University. His research interests are in membrane separation and nanofluidics by porous framework materials.

Mechanism and active sites of oxygen reduction reaction on nitrogen-doped carbon catalysts

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Polymer electrolyte fuel cell (PEFC) is a promising energy converter for the next generation. However, the high cost of platinum used in fuel cells, especially in the oxygen reduction reaction (ORR), is a major challenge. Carbon catalysts are expected to be used as electrode catalysts to replace platinum, and research has become explosively active. Among carbon catalysts, nitrogen-doped carbon catalysts for ORR are attracting particular attention. However, it was unclear which nitrogen species, graphitic nitrogen (grap-N) or pyridinic nitrogen (pyri-N), forms the active sites. We have revealed that pyri-N forms active sites using highly oriented pyrolytic graphite (HOPG) model catalysts in which grap-N or pyri-N is selectively doped1,2). Furthermore, we investigated the role of pyri-N in the ORR reaction mechanism using model catalysts in which pyri-N-containing molecules such as 1,10 phenanthroline molecules were supported on carbon black3). XPS measurements revealed that the pyri-N is converted to pyridinium ion (pyri-NH$^+$) in acid electrolytes, indicating its role as a proton adsorption site. Interestingly, it was found that the O_2 molecules is adsorbed upon the reduction of pyri-NH$^+$ to pyri-NH. That is, the thermal reaction O_2 adsorption is coupled with electrochemical reduction of pyri-NH$^+$ to pyri-NH.

$$\text{pyri-NH}^+ + O_2 + e^- \rightarrow \text{pyri-NH} + O_{2,a}$$

DFT calculations explain that an electron used for reducing pyri-NH$^+$ is introduced into π^* of the graphite system and an O_2 molecule adsorb on the carbon atom with its radical electron3,4). Furthermore, since pyri-NH$^+$ is hydrophilic, the equilibrium potential in the above equation decreases when it becomes hydrated and stabilized. This is the reason why the activity of nitrogen-doped carbon catalysts is low in acidic electrolytes. Therefore, in catalyst design, it is important to maintain hydrophobicity near the active site2-4).

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Junji Nakamura received received his doctoral degree from Hokkaido University in 1988. After postdoctoral work at Indiana University and University of Washington, he joined University of Tsukuba as a Lecturer in 1990 and was promoted to Associate Professor and Professor in 2006. In 2022, he retired from University of Tsukuba and moved to Kyushu University. He has performed surface science studies combined with heterogeneous catalysis for over 40 years.

A Platform to Make and Un-Make Polymers: A Step Toward a Circular Carbon Economy

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Polymers are critical in nearly every aspect of human life. Polymers are used in our medical devices and personal protective equipment, vehicles, construction materials, electronic devices, packaging, our clothes and more. Unfortunately, we do not make polymers sustainably. Most polymers are manufactured from non-sustainable feedstocks, used for a limited time, and then discarded in landfill or incinerated. Humans have made a staggering 8 billion tonnes of plastic and less than 10% has been recycled.[1] Of the relatively small fraction of polymers that are recycled, this is typically achieved through thermomechanical processing that ultimately degrades the material. For this reason, new platform technologies are needed so that polymers can be generally recycled and converted back into monomer building blocks.[2] Such *chemical recycling* strategies will be necessary for a circular carbon economy.[3]

In this lecture, I will present two case studies on making polymers that can be chemically recycled. Both polymers feature a trisulfide linkage incorporated throughout the backbone that serves as a trigger for selective and rapid depolymerisation after the polymer has served its function. The first case study centres on the electrochemical or photochemical ring-opening polymerisation of cyclic trisulfides. These sulfur-rich materials have found use in gold mining and e-waste recycling, where the polymer serves as a recyclable gold sorbent.[4] The second case study features a novel and rapid S-S metathesis reaction unique to linear trisulfides.[5] This unusual chemistry can be used to make recyclable analogues of polyolefins, polyurethanes, polyamides and more. Prospects in the use of this novel chemistry as a platform for chemically recyclable polymers will be discussed.

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Presenter's Biography

Justin Chalker is an ARC Future Fellow and Matthew Flinders Professor of Chemistry at Flinders University in Adelaide, South Australia. He completed his undergraduate studies at the University of Pittsburgh (USA), where he was trained in organic chemistry and completed the total synthesis of multiple natural products under the supervision of Prof Theodore Cohen. Justin then moved to the UK as a Rhodes Scholar and completed his D.Phil. at the University of Oxford under the supervision of Prof. Benjamin Davis. At Oxford, Justin developed several novel and selective methods for the covalent modification of proteins. Upon completing his D.Phil., Justin started his independent laboratory at the University of Tulsa in 2012 and then moved to Flinders University with the support of an ARC DECRA in 2015. Justin's current research interests span polymer chemistry, sulfur chemistry, and applications in environmental protection and sustainability. Justin's research has been recognised with several awards including the 2020 Prime Minister's Prize for New Innovators, one of the top science prizes in Australia.

Engineering nanobiohybrids for environmental sustainability

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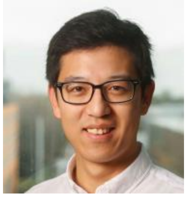
Nanobiohybrids, synthesized by integrating functional nanomaterials with biological systems, have emerged as an exciting branch of research at the interface of materials engineering and biological science. Nanobiohybrids use synthetic nanomaterials to impart organisms with emergent properties outside their scope of evolution. Consequently, they endow new or augmented properties that are either innate or exogenous, such as artificial photosynthesis, conductivity, enhanced tolerance against stress, or programmed metabolism and proliferation.

In this talk, I will highlight some of our recent efforts in the design and engineering of open framework material based nanobiohybrids for sustainable engineering applications, to address emerging challenges in the environment, energy, and biomedicine.

Presenter's Biography

Kang Liang obtained his Ph.D. in Chemical and Biomolecular Engineering from the University of Melbourne in 2014. He is a Fellow of the Royal Society of Chemistry and an Australian Research Council Future Fellow. He currently serves as a Scientia Associate Professor in the School of Chemical Engineering and the Graduate School of Biomedical Engineering at the University of New South Wales, Australia.



True surface SEM imaging of carbon materials at ultra-low acceleration voltages below 1 kV

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Scanning electron microscopes (SEM) are a workhorse tool in carbon material research. They offer high-resolution images that reveal the surface features, composition, and crystallographic information of these materials. This information is crucial for understanding how carbon nanotubes, graphene, fibers, and other materials are formed and how they perform. From characterizing the size and quality of carbon nanotubes to examining the pore structure of activated carbon, SEM helps researchers design and develop new and improved carbon materials for various applications. However, imaging of these carbon materials if often challenging due to their small dimensions which causes electron transparency. Further, there is the possibility that the electron beam damages the structure of the material. These challenges can be overcome by using low or ultra-low acceleration voltages below 1 kV. However low or ultra-low kV SEM imaging presents its own challenges which include: (i) Poor signal-to-noise ratio; (ii) Low image resolution and (iii) Image distortion due to poor alignment of low energy beam. We will show how latest developments in Gemini SEM column design enable sub-nanometer resolution imaging on beam sensitive, non-conductive and magnetic surfaces at low and ultra-low kV.

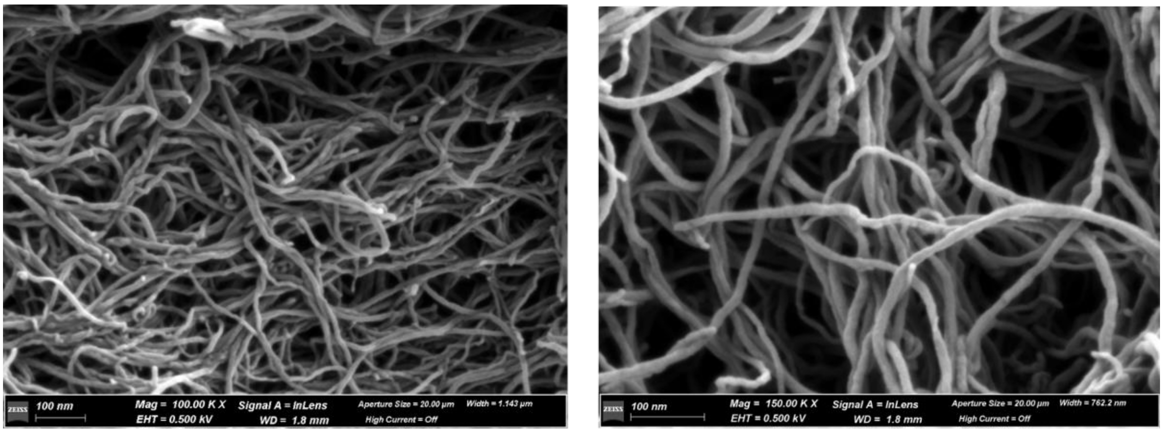

Figure 1: High resoltuon surface topography of carbon nanotubes (CNTs), imaged with an acceleration voltage of 0.5 kV

Kashmira Raghu is part of the ZEISS Australia and New Zealand team and looks after the electron and xray microscopy business in Australia. Kashmira Raghu is an experienced sales specialist in electron microscopy, with a focus on providing high-quality solutions to customers. With over 10 years of experience in EM, Kashmira has a deep understanding of the technology and its applications across various industries.

Development of advanced Li-ion batteries and beyond to reduce cost and ensure sustainability for electric vehicles.

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To meet the high-energy requirement that can enable the 40-miles electric drive Plug in Hybrid Electric Vehicle (P-HEVs), long range electric vehicle (EV) and smart grid, it is necessary to develop very high energy and high-power cathodes and anodes that when combined in a battery system must offer over 1,000 charge-depleting cycles, 15years calendar life as well as excellent abuse tolerance. These challenging requirements make it difficult for conventional battery systems to be adopted in P-HEVs and EVs. In this talk, we will first introduce the next generation lithium-ion battery that include Ni rich full gradient cathode with Nano-rode primary particles, a novel advanced PEDOT coating to extend the calendar life of battery, a high voltage and non-flammable Fluorinated based electrolytes and Silicon-graphene composite anode including a novel pre-lithiation technology to overcome the irreversible loss of this anode in the first cycle. We will then finish by describing a novel Lithium superoxide close system that offers at least 2 times more energy density than state of the art lithium ion.

Presenter's Biography

Dr. Khalil Amine is an Argonne Distinguished Fellow and the leader of the Advanced Battery Technology team at Argonne National Laboratory, where he is responsible for directing the research and development of advanced materials and battery systems for HEV, PHEV, EV, grid, satellite, military, and medical applications. Dr. Amine is also the Co-director of the US-German initiative on interface. He serves as a member of the US National Academy of inventors and fellow of the European academy of sciences and committee member of the U.S. National Research Consul at US Academy of Sciences on battery related technologies. He served until recently as an adjunct professor at Stanford University and held a joint appointment as Professor at the University of Chicago. Among his many awards, Dr. Amine is 2023 recipient of Kuwait prize, 2019 recipient of the mega global energy prize, a 2003 recipient of Scientific America's Top Worldwide 50 Researcher Award, a 2009 recipient of the US Federal Laboratory Award for Excellence in Technology Transfer, 2013 DOE Vehicle technologies office award and is the six-time recipient of the R&D 100 Award which is considered as the Oscar of technology and innovation. In addition, he was awarded the ECS battery technology and battery research awards, the international battery association award and NAATB lifetime achievement award. Dr. Amine holds 207 patents and patent applications and has 776 publications with google h-index of 174. From 1998-2022, Dr. Amine was the most cited scientist in the world in the field of battery technology with over 104,500 citations. He serves as the executive director and vice president of IMLB. He is also the chairmen of the international automotive lithium battery association, ECS fellow, Fellow of the international association of advanced materials, and associate editor of the journal of Nano-Energy.

Multiscale Design of Carbon-Based Catalysts: A Maximum Entropy Production Approach using Reaction-Diffusion Dynamics

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We explore a novel theoretical approach for spatio-temporal pattern forecasting based on a reaction-diffusion formulation. The approach provides a theoretical basis for future deep learning models and multiphysics upscaling of the catalyst's molecular dynamics and density functional models across multiphysics fields. We first investigate the Schrödinger-bridge transport problem as an analogy for the uncertainty of the ground state for rational catalysis design. Then, we show that through the Maximum Entropy Production assumption of the interaction between the catalyst and the target molecule, we arrive at the most probable nonlocal dynamic equilibrium of the catalytic reactions[1]. We then investigate two specific cases: patterns that develop in a system far from equilibrium yet maintaining local equilibrium and patterns that form under conditions of nonlocal equilibrium. We posit that through this approach the design of new carbon-based catalysts is possible.

We apply the novel approach to explore nature's principle of reaction-motion coupling of enzymes or higher-order organisms such as cyanobacteria (Fig. 1) that act as carriers of catalytic pigments (chlorophyll). These bacteria operate as “active matter” where individual bacteria actively consume energy through their collective motion leading to complex, large-scale self-propelling motions. This implies that the catalyst surface is not an unchanging energy landscape but can change dynamically over time and space. We show that the dynamic equilibrium approach defines a set of patterns that optimizes the catalytic reaction based on the properties of multiscale reactions and diffusion. A nonlocal reaction-cross-diffusion formulation of catalytic reactions captures the interaction of the catalyst with the target molecule.

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Regenauer-Lieb, K. & Hu, M. (2023), Heliyon, ***9,12,*** *DOI:10.1016/j.heliyon.2023.e22701*

Figure 1: Cyanobacteria consume CO_2 to produce carbonaceous equidistant columnar structures (microbialites) that form a typical Turing pattern by catalytic reaction diffusion processes. They live in highly saline waters and release oxygen in bubbles floating on the water surface. Catalytic reactions incorporate the effect of coupling to fluid flow visible by the preferential advection of the bubbles in the direction of prevailing wind (diagonal to the top right). Mature microbialite collonies (not shown) maximise oxygen production through orienting growth along the prevalent wind.

Presenter’s Biography

Klaus Regenauer-Lieb is a geophysicist and applied mathematician with more than 30 years' experience in Renewable Energy and Reservoir Engineering. As Postdoctoral researcher he worked at the University of Minnesota, the Swiss ETH Zurich and CSIRO. He subsequently held Professor positions at the Johannes Gutenberg University, the University of Western Australia, the University of New South Wales and Curtin University. He is well-known in the field of mathematical solid and fluid dynamics having pioneered new techniques for multi-scale, multiphysics modelling of porous media based on fundamental physics, including the link between Earth's heat, its chemistry and its mechanical behaviour.

Strategies for Achieving Carbon Neutrality in the Chemical Industry

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This study explores the diverse strategies chemical companies are employing to achieve carbon neutrality amid escalating environmental regulations and societal demands for sustainability. The analysis highlights the integration of advanced technologies, process optimization, and the shift towards sustainable raw materials, with a particular focus on the role of Carbon Capture and Storage (CCUS) technologies, renewable energy sources like wind, solar, and bio-based fuels, and the development of bio-based alternatives. These strategies aim not only to reduce the chemical sector's substantial carbon footprint but also to contribute to a broader sustainability agenda. Central to this investigation are the evaluations of CCUS technology and renewable energy integration, which are crucial for direct CO2 emission mitigation and reducing dependency on fossil fuels. The study further examines how enhancements in process efficiency and the adoption of more sustainable raw materials contribute to lower carbon footprints and less waste during production. Illustrated through successful case studies, this research showcases leading chemical firms that have made significant progress toward their carbon neutrality goals, such as those implementing CCUS technology to substantially decrease operational emissions. The discussion includes industry-wide challenges and opportunities, such as regulatory pressures and technological advancements, that influence these carbon reduction strategies. Overall, the findings provide actionable insights for chemical companies seeking to navigate their pathway to carbon neutrality and inform policymakers on creating supportive frameworks to facilitate this transition, underscoring the chemical industry's pivotal role in global sustainability efforts. Figure 1, is a detailed strategy diagram that outlines the necessary phases and methods to achieve carbon neutrality in the chemical industry:

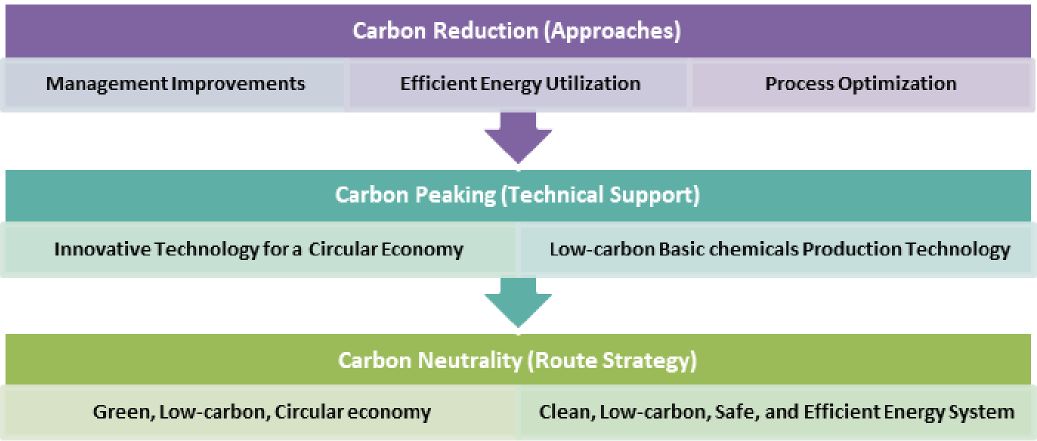

Figure 1 strategy diagram of the necessary phases and methods to achieve carbon neutrality in the chemical industry

Presenter's Biography

Ladan Malehmirchegini is a postdoctoral researcher at the International Institute for Carbon Neutral Energy Research (I2CNER), with a PhD in Energy and Environmental Engineering from Kyushu University. My research focuses on energy systems, environmental impact assessments, and optimization, with a particular interest in advancing carbon-neutral technologies. My graduate work, published in Science, explores innovative interdisciplinary approaches for the implementation of Smart Grid and Demand Response Technologies in the future electricity market. I have extensive experience in renewable energy systems, carbon capture and storage, and the design and optimization of advanced energy systems. I have published several papers in reputable journals and presented my work at international conferences. Recently, I have been developing pioneering assessment tools to evaluate carbon reduction potential in the chemical industry, a role that combines technical expertise with a deep understanding of the economic aspects of carbon-neutral technologies, preparing me to contribute effectively to projects aimed at optimizing carbon reduction processes.

Design of microtubular gas diffusion electrodes for gas-phase electrolysis

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Electrolysis of small gaseous molecules (e.g., CO_2, CO, NO) into value-added products and storing renewable electricity have drawn growing attention due to their zero-emission process and ability to operate at ambient conditions. In addition to effective electrocatalyst design, the design and configuration of the electrode are crucial for enhancing mass transportation and accelerating reaction kinetics. Traditional planar electrode suffers from low solubility of reactive gas and limited mass transportation when gas is bubbled into the catholyte. Recently, porous metallic hollow fibre gas diffusion electrodes (HFGDEs) with small radial dimensions have been emerging for the application of electrolysis due to several merits, such as a high specific surface-to-volume ratio, ease of fabrication, tailoring features, etc.

This work covers our recent design and fabrication of metallic Hollow fibre GDEs (HFGDEs). Various strategies, including in-situ alloying, catalyst nano-engineering, enhanced CO_2 distribution and reaction zone regulation, have been applied in electrochemical CO_2 reduction reaction (CO2RR) to improve the product selectivity, performance stability, surface wettability, and boost the current density. The microtubular GDE configuration has also been extended to electrochemical CO reduction reaction (CORR) for C_{2+} products while addressing carbonation and CO_2 loss issues. These different strategies on HFGDEs demonstrated simultaneously enhanced reaction rate and product selectivity towards the application perspective.

Quantum ionics: ultra-low energy consumption of energy conversion/information transmission in biologic system

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Life system presents an ultralow energy consumption in high-efficiency energy conversion, information transmission and bio-synthesis. The total energy intake of human body is about 2000 kcal/day to maintain all our activities, which is comparable to a power of ~ 100 W. The energy required for brain to work is equivalent to ~ 20 W, while the rest energy (~ 80 W) is used for other activities. All in vivo bio-syntheses take place only at body temperature, which is much lower than that of in vitro reactions. To achieve these ultralow energy-consumption processes, there should be a kind of ultralow-resistivity matter transport in nanochannels (e.g., ionic, molecular channels), in which the directional collective motion of ions or molecules is a necessary condition, rather than the traditional Newton diffusion. Directional collective motion of ions and molecules are considered as ionic/molecular superfluid. The research of ionic/molecular superfluid will promote the development of neuroscience and brain science, develop quantum ionic technology, and produce a series of disruptive technologies.

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Presenter's Biography

Lei Jiang is a Professor at the Technical Institute of Physics and Chemistry, Chinese Academy of Sciences (TIPC). He is an academician of the Chinese Academy of Sciences, Academy of Sciences for the Developing World, National Academy of Engineering (USA), Australian Academy of Science, Academia Europaea and European Academy of Engineering. Prof. Lei Jiang has discovered and established the basic principle of the interfacial material systems with superwettability and extended them to successful innovative applications. His work has been followed by more than 1,400 research institutions in 100 countries around the world. He is the most original and influential scientist in the field of material science in China. Due to his contribution to the development of superwettability, he won the "TWAS Prize in Chemistry" in 2011, the Advanced Science and Technology Award of "THE HO LEUNG HO LEE FUNDATION" in 2013 and the "Outstanding Achievement Award" of the Chinese Academy of Sciences in 2014. In 2016, he won the "UNESCO Medals" for contributions to the development of nanoscience and nanotechnologies, and the "Nikkei Asia Prize". In 2017, he won the "Humboldt Research Award" in Germany. In 2018, he was awarded the "Qiu Shi Outstanding Scientist Award" and "Nano Research Award". In 2020, he won the "ACS Nano Lectureship Award". In 2022, he won Tan Kah Kee Science Award.

The application of silicon anode materials in energy storage systems

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The Si-based materials have been extensively studied as anodes for lithium-ion batteries (LIBs). A key challenge for Si-based anode materials is their poor cycling stability, which is mainly due to the significant volume expansion that occurs during lithiation. To address this issue, an effective strategy has been developed that involves creating void spaces within the material structure to accommodate the volume changes. Among these strategies, yolk-shell Si/C structures have been shown to significantly improve the cycling performance of LIBs. In this report, promising structural optimizations aimed at further enhancing the overall performance of silicon-based anode materials will be presented. Additionally, advanced and simplified fabrication methods will be discussed.

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Biography

Dr. Lei Zhang earned his PhD from the Institute for Superconducting and Electronic Materials at the University of Wollongong, Australia. He is currently a DECRA Fellow at Griffith University. His research focuses on developing high-performance rechargeable batteries, recycling electrode materials from spent batteries, and integrating in-situ TEM technology into battery research.

2D Bi-based Nanomaterials for Clean Energy and Catalytic Applications

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Owing to unique structures and properties, 2D layered materials have exhibited great potentials for catalysis for clean energy and environmental sustainability. Among these, 2D Bi-based layered materials possessing intriguing characteristics have attracted tremendous attention. However, practical applications of these Bi-based semiconductors in catalysis remain a challenge due to their low catalytic efficiency. In most cases of them, the large band gap and unsuitable band-energy positions in band structures can lead to limited visible-light absorption and low solar-conversion efficiency. Additionally, the low concentration of active sites on the exposed accessible surfaces is also a key factor limiting their catalytic efficiencies. In this talk, I will present my recent research progresses on developing structural engineering strategies to overcome these limitations, including constituent adjustment, vacancy engineering, and construction of 2D hetero-structures.[1-6]

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Presenter's Biography

Dr. Liang Jason Wang is a GU Postdoctoral Fellow at the Centre for Catalysis and Clean Energy (CCCE) at Griffith University. He obtained his Ph.D. from the Institute for Superconducting and Electronic Materials (ISEM) at the University of Wollongong (UOW) in 2020. His research focuses on designing 2D layered nanomaterials for electro-catalysis and photo-catalysis, especially for energy conversion and environmental remediation. He has published over 50 peer-reviewed papers in high-impact journals with a *h*-index of 28, such as *Chem*, *Trends in Chemistry*, *Advanced Materials*, *etc*.

Catalyst Design for Optimal Urea Electrosynthesis

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Urea electrosynthesis under mild conditions presents a promising alternative to the harsh industrial Haber-Bosch process, which is hindered by sluggish C–N coupling and low selectivity. In this work, we leverage density functional theory simulations to propose several innovative strategies and mechanisms that harness the synergistic effects of N≡N bond cleavage and C–N coupling for highly efficient urea production.

Using CO and N_2 as feedstocks, we design dual vanadium atoms anchored to defective graphene (V_2N_6) to activate the adsorbed $*N_2$, serving as an effective catalyst for urea synthesis. In this system, the stable N≡N bond is gradually weakened and ultimately cleaved after two protonation steps, demonstrating superior thermodynamic and kinetic feasibility. Additionally, we explore an alternative pathway in which a free CO molecule is inserted into dimerized $*N_2$, binding concurrently with two nitrogen atoms to form a specific urea precursor, *NNCONN*. Our proposed mechanism identifies $Ti_2@C_4N_3$ and $V_2@C_4N_3$ as highly active catalysts for electrocatalytic urea formation.

To further enhance the efficiency, we also design dual reaction centre catalysts with two spatially independent active sites, each dedicated to a critical reaction step, using a 2D MOF framework, inspired by the concept of an automobile assembly line.

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Biography

Liangzhi Kou is currently an Associate Professor at Queensland University of Technology in Australia. He obtained his PhD from Nanjing University of Aeronautics and Astronautics in 2011. He was a recipe of Humboldt Fellow (2012-2014) and DECRA fellow (2015-2018). Professor Kou's research primarily focuses on the computational discovery and design of 2D materials for novel energy applications and electronic devices. He has published over 180 papers in top journals, including *Nature Communications*, *JACS*, *Nano Letters*, and *Advanced Functional Materials*, with more than 12,000 citations and an h-index of 58.

Oral Presentation

(Scope: 1. Nanostructured Materials)

Perovskite Quantum Dots for Solar Cells and Beyond

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Halide perovskite solar cells have witnessed great successes recently while their instability is a big hurdle for practical application. Herein we discuss our recent progress in addressing the stability of perovskite solar cells, including introduction of capping layers to improve the stability against moisture and heat, and perovskite size engineering to suppress phase segregation. In particular, quantum dots (QDs) have the advantages of quantum confinement effect, defect-tolerant nature, and processability for flexible devices. We discuss a new colloidal surface ligand engineering strategy in designing new hybrid perovskite QDs with controllable compositions and sizes The QDs have been used as building blocks in quantum dot solar cells delivering a certified record efficiency of 16.6% with excellent long-term operation stability. By using QDs as light absorbing materials, the QD based photocatalysts also exhibited good stable performance in photocatalytic hydrogen production. The combination of perovskite QDs with Metal-Organic Framework (MOF) materials to form new composites led to ultrastable photoluminescent property for > 10,000 hours. The integration of perovskite solar cells and rechargeable batteries have led to a single module type rechargeable solar batteries with an overall storable solar energy conversion efficiency of >12%.

Advancing Electrochemical N_2 Reduction: Interfacial Electrolyte Effects and *Operando* Computational Approaches

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Ammonia (NH_3) is a carbon-free energy carrier and is essential in agriculture and food industries. More than 95% of NH_3 production relies on the traditional Haber-Bosch process that is energy intensive with significant greenhouse gas (*i.e.* CO_2) emission because of intensive processing conditions such as temperature of 400-600 °C and pressure of 20-40 MPa.[1] Electrochemical N_2 reduction reaction (eNRR) is a promising alternative for sustainable and carbon-free green NH_3 synthesis (gNH_3s) due to the increasing level of renewable energy and abundance of N_2. However, further development is necessary to achieve cost and efficiency competitiveness with the traditional Haber-Bosch process.

Atomic-level investigations reveal that a key challenge for eNRR is the limited accessibility of N_2 molecules at the electrode interface, as resulting in low N_2 coverage and reduced selectivity.[2] To address this, research has shifted from traditional catalyst design to modulating the microenvironment at the electrode-electrolyte interface (EEI), yielding promising practical results. Currently, two promising eNRR strategies have emerged: (1) direct electrocatalytic N_2 reduction on electrode surfaces and (2) alkali metal-mediated N_2 reduction (AM-NRR).[3,4] Optimizing electrolyte composition is critical, with promising results from cation screening, solvent selection, ionic liquids, and alkali metal (e.g., lithium, and calcium) mediation.[4,5]

Emerging *operando* computational techniques to that incorporate precise static description of realistic electrochemical conditions (i.e. electrode potential and pH), and/or the timescale, achieved by the kinetic modelling (mean field – microkinetic modelling and kinetic Monte Carlo simulation), *ab initio* modelling incorporated with explicit solvent molecules and machine learning-interatomic potential (ML-IAPs) for extended simulation time-scales. These advanced techniques enable us to conduct simulations not only for material design but also for capturing interfacial dynamics, which is crucial for advancing electrolyte design modelling in complex scenarios.[6,7] Therefore, further design based on integration of material regulation and electrolyte engineering appears practical for realization of gNH_3s.

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Presenter’s Biography

Lin Jiang is a PhD candidate in School of chemical engineering at the University of Adelaide, specializing in theroretical computation and modelling in electrocatalysis. Lin’s research focuses on theoretical insights and computational approaches to electrochemical nitrogen reduction reactions (eNRR). Her work aims to uncover novel strategies to enhance catalytic performance using alkali metals and optimize electrolyte composition for sustainable ammonia synthesis.

Regulation of Electrochemical Active Sites *via* Carbon Microstructure

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Dual-metal-atom (DMA) catalysts with a wide variety of combinations have been developed to further enhance the catalytic activity of SMA catalysts through synergistic effects, especially for multi-step catalytic reactions. Due to the lack of the level of molecular design, two metal atoms generally tend to be randomly distributed in the resultant carbon skeleton by traditional calcination method. Besides, the high-temperature pyrolysis also leads to the thermal migration to induce random distribution and agglomeration of metal atoms, and thus the relatively poor DMASs configuration and low metal loading. Here, a molecular-design and carbon dot-confinement coupling strategy through the pyrolysis of bimetallic complex of diethylenetriamine pentaacetic acid under low-temperature is proposed as a universal approach to dual-metal-atom sites in carbon dots (DMASs-CDs). CDs as the "carbon islands" could block the migration of DMASs across "islands" to achieve dynamic stability. More than twenty DMASs-CDs with specific composition of DMASs (pairwise combinations among Fe, Co, Ni, Mn, Zn, Cu, and Mo) have been synthesized successfully. Thereafter, high intrinsic activity is observed for the probe reaction of urea oxidation on NiMn-CDs. In-situ and ex-situ spectroscopic characterization and first-principle calculations unveil that synergistic effect in NiMn-DMASs could stretch urea molecule and weaken the N-H bond, endowing NiMn-CDs with a low energy barrier for urea dehydrogenation. Moreover, DMASs-CDs for various target electrochemical reactions, including but not limited to urea oxidation, are realized by optimizing the specific DMAS combination in CDs.

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Metallated Graphynes: Synthesis, Characterization, and Optical and Catalytic Properties

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The doping and anchoring of single-metal atoms into graphdiynes (GDYs) can tune their electronic structure and broaden the usage. Herein, metal elements as a new functional units can be introduced into the frameworks of GDYs via metal-alkyne bonds to afford novel metallated GYs (MGYs). However, related research work is still in its infancy and their large-area and free-standing nanosheets were first isolated for use in the optical devices and catalysis by us in 2021.The novel MGYs has been designed and synthesized with homo- or hetero-metallic skeleton via the facile bottom-up method, which integrates the advantages of both metal centers and graphyne frameworks. The propensity of d_{10} Hg(II)-, d_8 Ni(II)-, Pd(II)- and Pt(II)-$(PR_3)_2$ (R = alkyl chain) units to form a moiety with alkynyl units makes them attractive building blocks for 2D organometallic functional materials. Both few-layer and multi-layer 2D nanosheets can be generated depending on the types of interface-assisted (i.e. liquid/liquid and gas/liquid) approaches and their bulks can be prepared by the one-pot method. The ligand structures and electronic properties can be easily adjusted in terms of the spacer length between the ethynyl unit and central core, central chromophore as well as the number of coordination sites. Therefore, the 2D nanosheets with different topological structures, pore sizes, surface areas and advanced functionalities can be prepared by using different monomers with diverse electronic, optical and catalytic properties. The relationship between the performance of MGYs and their well-defined nanostructures will be elucidated, with a major focus on studying the effects of transition metals and ligands in activating their optical and catalytic properties. The properties and catalytic performance can be fine-tuned through chemical modification of the chromophores. The proposed work can produce a new class of 2D carbon-rich materials and provide a design concept for developing efficient nonlinear optical materials and photo-/electro-catalysts.

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Presenter's Biography

Dr. Xu Linli is currently an assistant professor in the Department of Applied Biology and Chemical Technology at the Hong Kong Polytechnic University. Mainly focus on 2D carbon and carbon rich materials and their applications in the fields of optoelectronics, energy science, memory storage, and thermal management. She has published over 40 papers in important academic journals such as *Chem. Soc. Rev.*, *J. Am. Chem. Soc.*, *Agnew. Chem. Int. Ed.*, *Nano Today*, *Coord. Chem. Rev.*, led 10 projects, Participated in 9 funding projects, wrote 3 monographs, and authorized 8 national invention patents.

Hierarchical nanostructures for high performance electrocatalysis

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The development of improved and lower cost electrode materials is critical to produce cheaper, cleaner and more reliable hydrogen fuel for use in hydrogen fuel cell powered vehicles. Significant research has focused on improving catalysts, but support materials have received very little attention: The support determines how reactants, products and electrons move between the environment and the cell to create an effective device.[1,2] This work will present syntheses for 3D metal structures with dimensions on the nanoscale,[3] which can theoretically enable up to 1000 times greater efficiency than the current state-of-the-art supports. Developing chemical syntheses that directly grow metal cores and branches in sequential steps produces interconnected structures with controlled configurations that can be optimised for energy storage reactions (Figure 1). These materials have high surface area, high conductivity, and surfaces that can be chemically modified, which are properties that make them ideal electrocatalyst supports. This work introduces a synthetic concept to produce a new type of high-performing electrocatalyst support.

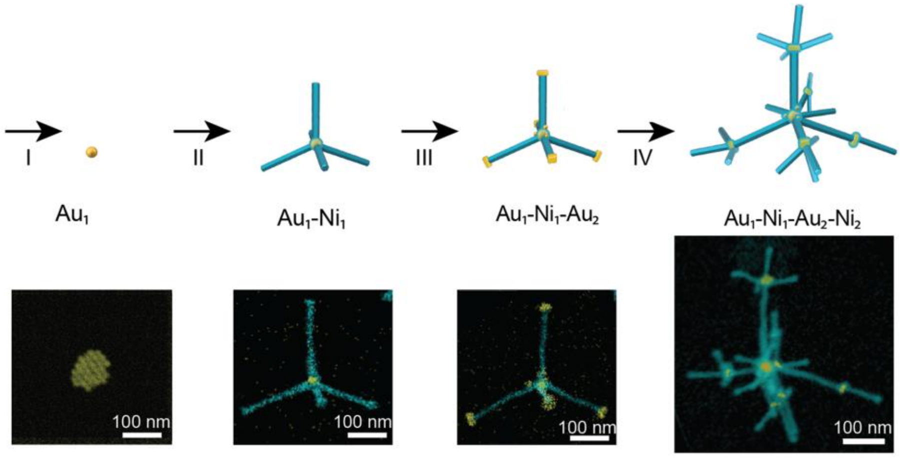

Figure 1: Synthetic approach for creating 3D nanostructures through iterative growth of Au cores and Ni branches.[3]

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Presenter's Biography

Lucy Gloag completed her PhD at the University of New South Wales in 2018 on the synthesis and characterisation of Ru-based nanocatalysts, before the commencement of her Postdoctoral Fellow positions. Her work on nanomaterials for electrocatalysis led her to an appointment as a Lecturer at the University of Technology Sydney in 2023. She joined the Research School of Chemistry at the Australian National University in 2024 to develop single atom and nanomaterials for energy storage and conversion technologies.

Boosting Solar-Driven Hydrogen Peroxide Production: Hydrophilic Engineering of Functionalized D-A Linear Polymers

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As an essential and versatile chemical, hydrogen peroxide (H_2O_2) has attracted numerous attentions and been widely applied in different areas, including disinfection, bleaching, and organic synthesis.[1, 2] Compared to conventional industrial process, the emerging route of photocatalytic H_2O_2 production from water and O_2 or air under the sunlight illumination provides a more environmentally friendly and economical solution.[3] Organic materials have shown great potential as photocatalysts for solar-driven H_2O_2 production owing to the advantages of structural diversity and flexibility.[4] However, many polymers suffer from the poor dispersibility in pure water, which greatly suppressed their photocatalytic performance. In this study, a facial strategy was introduced to improve the hydrophilicity of a donor–acceptor linear polymer (DE-AQ) via post-modification. The carboxyl group functionalized polymer, DE-AQ-COOH, exhibited significantly enhanced activity for photocatalytic H_2O_2 production, achieving a high rate of 4291.9 μmol g^{-1} h^{-1} and an apparent quantum yield (AQY) of 10.5%, which outperformed most reported organic photocatalysts. These findings highlight the potential of functional-group engineering as an effective approach for the development of highly efficient organic polymer-based photocatalysts.

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Presenter's Biography

Lunjie iu is a postdoctoral researcher in the Faculty of Engineering at the University of New South Wales (UNSW). He earned his Ph.D. in Chemistry from the University of Liverpool in the United Kingdom, where he specialized in developing polymer materials for energy conversion and storage applications. Currently, Dr. Liu's research focuses on innovative polymer and carbon-based materials, with projects aimed at advancing photocatalytic hydrogen peroxide (H_2O_2) production and developing sustainable methods for plastic waste recycling. His work seeks to address critical challenges in renewable energy and environmental sustainability, contributing to the development of cleaner, more efficient chemical processes.

Sustainable Batteries and Electrocatalytic Processes

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Batteries will continue to play a vital role in decarbonising transportation as well as in storing the intermittent renewable energy. Diversification of battery technologies with more sustainable options in mind, not only for the raw minerals but also for more sustainable manufacturing practices for cells and packs are needed. In my talk I will touch on some of these sustainable practices needed to be implemented today, while showing the 12 principles of “green batteries” inspired from “green chemistry” my research group introduced. I will then focus on Na-ion batteries with emphasis on our research on hard carbon anodes to understand the fundamentals on Na ion storage using multiple characterization techniques coupled with electrochemistry. I will also discuss the importance and complexity of solid electrolyte interfaces in Na ion batteries and some perspectives on commercialisation from our group.

In addition to batteries, green H_2 is also a key energy vector helping our transition to net zero. I will present our research on new substates for electrocatalytic H_2 production based on biomass/plastic waste derivatives such as glycerol, ethylene glycol or 5-hydroxymethylfurfural with advantages of lower potentials where the biomass/waste oxidation reactions occur and the opportunity of producing other high value chemicals in addition to green H_2, helping a circular economy in the chemicals production sector.

Finally, I will touch on the use of H_2 in fuel cells for zero carbon electricity production. The sluggish reaction here is the oxygen reduction reaction happening at the cathodes requiring Pt catalysts which are scarce and expensive. I will present research on bioinspired catalysts based on Fe single atoms coordinated to nitrogen atoms doped on a conductive carbon matrix and their activity toward Oxygen Reduction Reaction emphasising the importance of determining the number of active sites and understanding the challenges hindering the stability of such catalysts.

Presenter’s Biography

Magda Titirici is a Chair in Sustainable Energy Materials at Imperial College London. Prior she has worked at Queen Mary University of London and the Max-Planck Institute of Colloids and Interfaces. She is well recognised for her research in sustainable carbon materials for energy storage and conversion applications particularly batteries beyond Li ion, biomass electrolysiis to H2 and high value chemicals as well as developing Pt free catalysts for the Oxydation Reduction Reaction in fuel cells. She is on the list oh Clarivate Highly Cited Researchers since 2018 , only 13 years past her PhD. She has won numreous awards and regognition for her research from Royal Society, Royal Society of Chemistry, Royal Academy of Engineering, Institute for Materials and Mines, latest being the Imperial College President Award for Excelence in Research. Magda leads a diveres and muktidisciplinary team of bout 40 people in the Departament of Chemical Engineering at Imperial.

Title: *Practical* Graphene Oxide membranes for molecular separations

Short Biography: Mainak Majumder is a professor in the Department of Mechanical and Aerospace Engineering of Monash University. He joined Monash as a lecturer in 2010 after his postdoctoral stint at Rice University, USA (2008-2010). He is the Director of the Australian Research Council's Research Hub on Advanced Manufacturing with 2D Materials (AM2D), and an Associate Director of the Monash Energy Institute. He and his team have taken fundamental scientific breakthroughs in Graphene materials from the laboratory to market, including products such as energy-efficient water filtration systems and energy storage systems to enable dissemination of IoT technologies.

Abstract

Membrane-based separation technologies have many advantages over traditional separation methods such as adsorption, and distillation in terms of energy- and cost-efficiency and modular deployment of technology. In practice, these advantages can be meaningfully harnessed only if advanced membranes with properties such as high permeance, tailorable selectivity [1-2], chlorine, pH and solvent resistance [3-4], low-fouling characteristics [1], long-term stability under operational conditions [5,6] alongside green and sustainable manufacturability [6] are demonstrated. In the last 7-8 years, our research group has taken rapid strides to realize these properties in membranes made from graphene-oxide, including scaled-up manufacturing in roll-to-roll approaches. In this talk, I will summarize this journey reflecting on our work including some aspects of translation to industry and future directions.

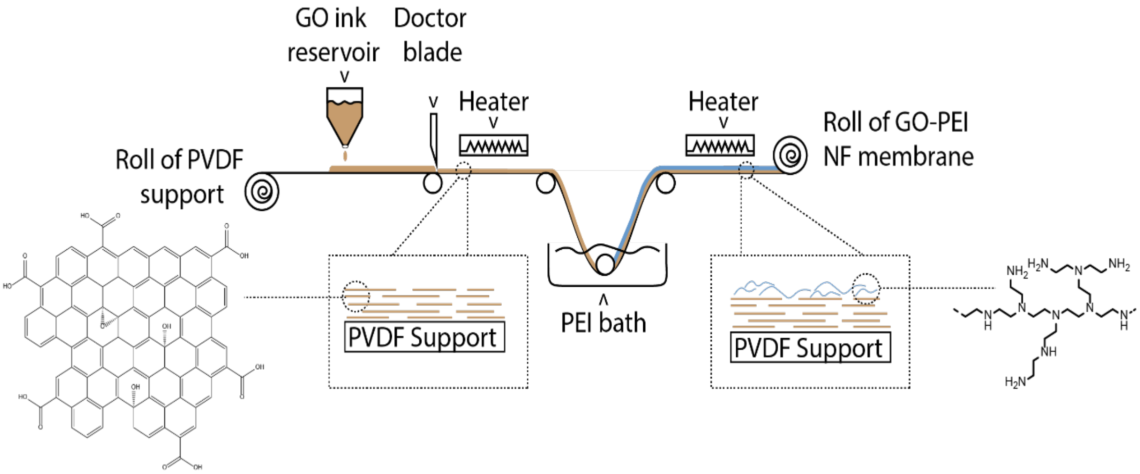

Figure 1: Schematic for roll-to-roll fabrication and modification of Graphene Oxide membrane. [5]

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Improved graphene oxide reduction using bimetallic core-shell Ag-Pt nanoparticles

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Surface plasmon resonance (SPR) presents compelling prospects for amplifying photocatalyst efficiency through the generation of "hot electrons" during surface plasmon decay. This holds the potential to elevate conversion yields in solar energy technologies[1]. However, there is a hitch in this process that the hot electrons tend to recombine with the holes. Extensive research is underway to investigate bimetallic photocatalyst nanoparticles, aiming to boost the mobility of these electrons towards active sites[2]. In our research, we endeavoured to provide evidence for this concept by reducing Graphene Oxide with visible and IR light. Under light exposure, the coupling of GO with Ag-Pt nanoparticles resulted in the highest observed conversion, as confirmed by UV-vis absorbance data, FTIR analysis, and conductivity measurements. This can be ascribed to the enhanced transfer of hot electrons from the plasmonic (Ag) nanoparticles to GO facilitated by the Pt islands.

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Presenter's Biography

Mrs Mani Mani, PhD scholar

Mrs Mani Mani is pursuing PhD from the School of Chemical Engineering, UNSW Sydney, in the field of Plasmonic Catalysis under the guidance of Dr. Priyank V Kumar. She is working with Ag nanoparticles in improving their activity by coating it with Pt and and even coupling it with semiconductor to evaluate their potential in specific applications. She has industrial experience of 7 years in petrochemicals sector where she has worked in Gas Cracker plant operations and commisioning of Pure Terephthalic Acid plant.

Nanoengineered Electroactive Polymers: A New Materials Paradigm for Neuromodulation

Matthew J. Griffith,[1] Rafael Crovador,[2,3] Paul C. Dastoor,[3] Alan M. Brichta,[2] Rebecca Lim[2]

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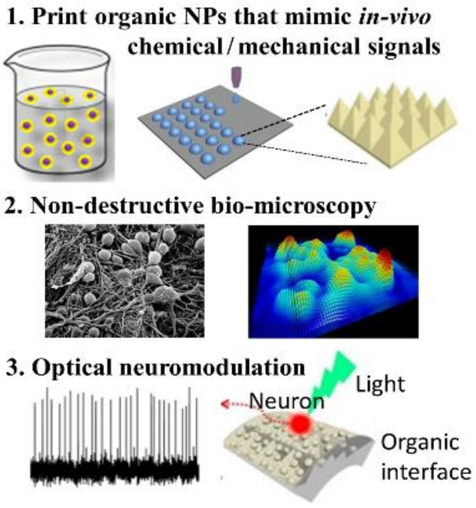
Communicating with the human body using carbon-based electronic devices is a grand challenge in materials science. In this talk I will discuss some highlights from our team's efforts to combine new electroactive polymer materials with nanoscale science and create bio-functional inks and printable devices that overcome the gap between the electronic and biological worlds.



Implantable neurostimulation devices have typically been fabricated with stiff electronic materials such as metals and silicon and thus progression out of the laboratory remains limited by low biocompatibility, a requirement for external power, and poor spatial resolution.[1] By combining soft carbon-based polymer inks with new bio-printing technologies[2] and establishing routes to incorporate neuroprotective drugs into these bio-inks,[3] our team established paradigm-shifting materials that combine electronic, chemical, and mechanical stimuli to communicate with biological cells in their natural language.
We demonstrated this potential by co-culturing retinal and ganglion neurons onto multi-functional electrodes fabricated from our nanoparticle inks, demonstrating both anatomical and functional biocompatibility via immunolabelling with neuronal marker MAP2 and visualization with epifluorescence microscopy. Finally, we employ whole-cell patch clamp electrophysiology recordings to demonstrate an exciting result; wireless neuromodulation of nerve cells via capacitive coupling which can be optimized by judicious selection of the device architecture.[4]

Our results have highlighted that nanoengineering electroactive polymers can overcome the gap between the electronic and biological worlds, enabling exciting new frontiers in health applications.

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Presenter's Biography

A/Prof Matthew Griffith studied chemistry, physics, and materials engineering at the University of Wollongong, graduating with a Bachelor of Nanotechnology in 2007 and a PhD in Chemistry in 2012. He then worked as a NEDO Fellow at Shinshu University in Japan, before returning to Australia and holding appointments as a post-doc and then Lecturer in Physics at the University of Newcastle (2013-2019), a Research Manager at the University of Sydney (2020–2023) and is currently an Associate Professor and ARC Future Fellow at the University of South Australia, where he leads the Centre for Nanoelectronic Materials and Devices. Matthew’s research focuses on developing innovative new carbon-based materials and devices that solve some of the biggest challenges facing humanity in the areas of Health and Energy. He is also the host of the Royal Australian Chemical Institute's official podcast, *Chemically Speaking*, and the Director of UniSA’s Microscopy and Microanalysis facilities.

Toward improved drug delivery via the bloodstream via tuning biomaterial affinity for the blood vessel wall

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Despite significant investment in biomaterials development for drug delivery, few have progressed to clinical use. Notwithstanding elegant biomaterials design, overcoming biological barriers *in vivo* remains a challenge. This is in part attributed to the disparity in the evaluation of biomaterials between *in vitro* and *in vivo* systems.

Fundamental to all mammalian cells are the cell membrane anchored glycan macromolecules which form an anionic hydrogel-like matrix, called the glycocalyx. Yet, few have considered the glycocalyx in either the design or preclinical testing of biomaterials. With most biomaterial drug delivery systems administered via the bloodstream, the blood vessel wall is a key tissue barrier to traverse on the path to target tissues. Thus, the endothelial cell glycocalyx is an important consideration in the design of biomaterials which are able to traverse the blood vessel wall[1].

We established an *in vitro* blood vessel model in which the glycocalyx is expressed by primary human endothelial cells. This model was used to assess the interactions of various carbon-based biomaterials in either molecular polymer or nanoparticle formats. Our analyses reveal that cationic and neutrally charged biomaterials possess higher levels of association with cells expressing a glycocalyx than anionic biomaterials[2]. Furthermore, we found that the glycocalyx promotes the internalisation of cationic biomaterials.

To gain further insight into the mechanisms of biomaterial-glycan interactions we tethered glycans to gold substrates via thiol chemistry enabling biomaterial interactions with these systems to be measured using the quartz crystal microbalance. This approach revealed that cationic biomaterials bind glycocalyx components via a condensation mechanism with the affinity of these interactions positively correlated with glycan sulphation. These findings suggest the ability to tune biomaterial transport through the glycocalyx via biomaterial-glycan affinity which presents new insights toward improved design of drug delivery systems.

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Presenter’s Biography

Megan Lord is a Professor in the Graduate School of Biomedical Engineering, UNSW Sydney. She attained a Doctor of Philosophy in Engineering, Master of Biomedical Engineering and First class Honours degree in Chemical Engineering from UNSW Sydney. Megan’s research centres on the engineering of cell-biomaterial interactions for applications in drug delivery and regenerative medicine. She is the recipient of numerous awards including an Australian Research Council Future Fellowship (2022) and the Barry Preston Award from the Matrix Biology Society of Australia and New Zealand (2022). Megan serves on the Standards Australia Committee HE-030 Biological and Clinical Evaluation of Medical Devices that reviews and ratifies ISO 10993 and TC 194. She has served as Presideint of the Matrix Biology Society of Australia and New Zealand and is the founding Academic Director of both the Molecular Surface Interaction Laboratory (Mark Wainwright Analytical Centre) and Industry PhD Program (Faculty of Engineering) at UNSW.

Fully Roll-to-Roll Fabricated High-Efficiency Thin Film Solar Cells

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Abstract

Solar energy, nature’s most abundant source of renewable energy, has become the focus of the transition to net-zero in the 21st century. In contrast to conventional silicon solar cell manufacturing process, the advancement of high-volume, low-cost roll-to-roll (R2R) printing techniques has revolutionized thin-film solar cell production. This technique involves the continuous deposition of the components of a solar cell onto flexible substrates using industry-ready coating methods, facilitating the production of lightweight, rollable, and high-efficiency solar cells while significantly lowering costs. The unique form factor of these solar panels also results in a high specific power (power-to-weight ratio), which is highly desirable for emerging applications, including space, drones, vehicle-integrated PV, and building-integrated PV.

In this talk, an overview of the latest developments in R2R printing technologies is presented. To bridge the significant efficiency gap between devices fabricated by lab-scale spin coating and scalable deposition methods, enormous efforts have been devoted to achieving reliable, pinhole-free, uniform films using the R2R deposition process. We have demonstrated the highest power conversion efficiency (PCE) for fully vacuum-free R2R-fabricated solar modules. A deep understanding of how the thin-film formation process impacts the quality of the printed film is highlighted, allowing for the identification of key problems and optimization of the deposition process so that these innovations can make an impact in the broader community.

Methylammonium-free inks for upscalable fabrication of perovskite thin films and solar cells

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Perovskite solar cells (PSCs) have been considered as one of the most competitive candidates for the next generation photovoltaics. The α-formamidinium lead iodide (α-$FAPbI_3$) perovskite has been dominating the high-efficiency perovskite photovoltaics, but it still relies heavily on multiple additives in upscalable film fabrication in air. Compared to methylammonium (MA)-based perovskite, the blade-coating fabrication of phase-pure α-$FAPbI_3$ in ambient air can be much more challenging. And high-quality crystallization of α-$FAPbI_3$ usually requires MACl as an additive. Howerver, the residual extrinsic ions of MA^+ is found detrimental to the long-term stability of the devices, which motivates us to explore blade-coating deposition of α-$FAPbI_3$ without any MA containing additives. This talk will cover our latest progress on developing the MA-free perovskite inks for upscalable fabrication of α-$FAPbI_3$ thin films. The discussion is focused on the colloidal precursor, intermediated phases and crystallization control of the gas-quenching perovskite ink employing different ligand and additives, showing the morphology-controlled device performance and stability of the gas-quenched FA-based perovskite solar cells as well as the principles for designing suitable inks for MA-free perovskite. The latest result on post-treatment for pinhole-rich perovskite films will be also reported.

Presenter's Biography

Dr. Meng Zhang is currently an ARC DECRA fellow at University of New South Wales. He obtained his Ph.D. at the University of Queensland in 2016, and joined University of New South Wales for postdoctoral research. He has been employed as a Professor in Southwest Petroleum University. His research interests include materials engineering for metal halide perovskite materials and stability evaluation of perovskite solar cells.

Development of carbon gas-diffusion electrodes for stable CO_2 electrolysis

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CO_2 electrolysis is a promising electrochemical route to convert waste CO_2 into useful products such as CO, C_2H_4, or ethanol. Research efforts over the past decades have greatly improved its reaction rate close to the industrially applicable rate through the use of carbon-based gas-diffusion electrodes, where the catalyst layers (CLs) are positioned at gas/liquid interfaces. This electrode configuration significantly shortens the transport distance for CO_2 to reach the catalyst surface and maximises the catalyst area available for CO_2 conversion. However, it also leads to severe electrode flooding or salt precipitation within the electrode that hinder CO_2 supply to the catalyst and thus reduce product selectivity and conversion efficiency. This talk will report our recent work to address this critical stability issue by tailoring the carbon electrode interfaces and catalyst layers.

Presenter's Biography

Dr.Mengran Li is a lecturer and ARC DECRA fellow at the Department of Chemical Engineering, University of Melbourne (UoM). After obtaining his PhD from the University of Queensland (UQ) in 2016, he spent over three years as a postdoctoral research fellow at UQ, working on developing CO_2 electrolysis technology for the iron and steel industry. In 2021, Dr.Li joined the Delft University of Technology in the Netherlands as a postdoctoral researcher. There, he continued his work on CO_2 electrolysis in collaboration with other European institutes and companies, supported by the EU Horizon Project SELECTCO2. He then joined UoM in 2023, the same year he was awarded the ARC DECRA fellowship. At UoM, Dr.Li is leading the Li Energy Lab, which focuses on advancing electrochemical technologies crucial for the global energy transition towards a greener future. His research includes CO_2/water electrolysis, reactive carbon capture, fuel cells, and hydrogen separation and compression.

Effect of Methoxy Substitution on the Stability of Cobalt Phthalocyanine Catalysts for CO_2 Reduction

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This study investigates the effect of methoxy substitution on cobalt phthalocyanine (CoPc) as a molecular catalyst for electrochemical CO_2 reduction reaction (CO_2RR), focusing on enhancing catalyst stability under high-current conditions. Previous research has shown that CoPc can undergo demetalation at elevated currents, compromising its catalytic efficacy, and that CO_2 binding at non-metal centers in similar catalysts, like CoTPP, can lead to carboxylation, further affecting performance.[1] By introducing methoxy groups, we aim to stabilize CoPc by leveraging the substituent's electron-donating effects to favor CO_2 coordination at the metal center.[2] This selective binding could mitigate side reactions at non-metal sites, enhancing long-term operational stability. Ultimately, this approach may provide insights into the design of CoPc-based catalysts with improved durability and selectivity in CO_2RR applications.

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Presenter's Biography

Mengxin Liu graduated with a Bachelor of Science from Jilin University, China, in 2023, and obtained a Master of Science from the National University of Singapore. She joined Macquarie University in 2024 to pursue both MRes and PhD programs. Her primary research focuses on CO_2 electrocatalysis, aiming to develop efficient CO_2 conversion technologies to address global climate challenges.

Organic Multi Exciton Generation Augmented Silicon (OMEGA)

M.P. Nielsen[1], P. M. Pearce[1], J. Beves[2], N. Chang[1], Y. Cho[1], A.J. Baldacchino[3], J. Tong[1], M.W. Brett[2], S. McNab[1], B.P. Carwithen[2], M.J.Y Tayebjee[1], N.J. Ekins-Daukes[1], J.Y. Jiang[1], B. Hoex[1], A.M. Ciesla[1], T.W. Schmidt[2], D.R. McCamey[3], M.J.Y Tayebjee[1], and N.J. Ekins-Daukes[1]

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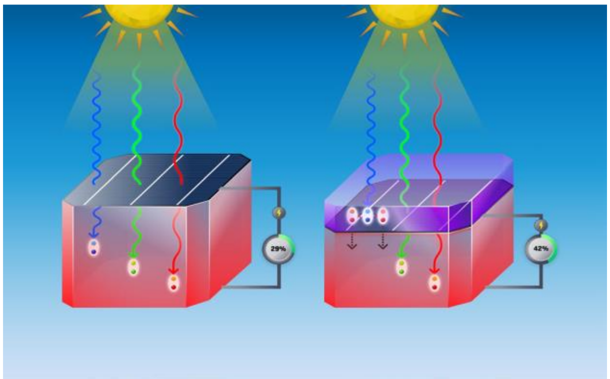

Figure 1: Singlet fission silicon tandem solar cells have the potential to be the next generation of photovoltaic technology.

Current silicon photovoltaics are approaching the single-junction efficiency limit, which is largely imposed by the inevitable thermalization losses caused as above-gap photocarriers relax to the band-edge prior to extraction. These losses could be mitigated if the excess energy of a photon could instead be used to produce an additional excitation, and organic molecular singlet fission has been touted as a highly efficient method of multi-exciton generation towards this goal. Harvesting the nascent triplets in a silicon cell via transfer across an appropriately designed interface could then lead to improved photocurrent. An alternative approach is to radiatively couple a chromophore to silicon via quantum cutting, wherein the absorption of a high-energy photon leads to emission of two down-converted photons closer to the silicon band gap. Here, I will discuss our efforts to design augmented silicon devices via singlet fission and/or optical down-conversion in novel sensitizer-interlayer-silicon architectures. Through magnetic field-dependent photocurrent and photoluminescence measurements, we reveal identify triplet transfer efficiencies into silicon solar cells. In addition our efforts in developing singlet fission enhanced silicon photovoltaics, I will discuss how charge and energy transfer at hybrid inorganic-organic interfaces can lead to new classes of optoelectronic devices.

Presenter's Biography

Dr Michael P. Nielsen is currently a Senior Lecturer in the School of Photovoltaic and Renewable Energy Engineering. He holds both a UNSW Scientia Appointment and an ARC DECRA Fellowship. His research is focused on using advanced characterisation techniques to understand and develop novel optoelectronic devices. This includes both the use of ultrafast spectroscopy to understand photovoltaic interfaces as well as develop alternative energy producing devices such as the mid-infrared thermoradiative diode.

Carbon capture for improving sustainability of urban water management

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The presence of carbon dioxide (CO_2) content (15–60%) in raw biogas is a major factor that lowers its caloric value and limits its application as an energy source. Although various techniques have been developed for adsorbing CO_2, the residual materials require disposal or regeneration, and the CO_2 released back into the atmosphere can potentially cause secondary pollution. Recent work proposes an integrated solution of upgrading biogas using an iron-electrochemical technology by storing carbon as solid carbonate mineral ferrous carbonate ($FeCO_3$) and directly applying the byproduct $FeCO_3$ to urban wastewater systems. Through long-term operation of two continuous-flow laboratory-scale urban wastewater systems, each consisting of sewer reactors, a sequencing batch wastewater treatment reactor, and an anaerobic digester, the results demonstrated that dosing $FeCO_3$ (10 mg Fe/L) in sewers can bring multiple benefits for urban wastewater management. As iron reacts with anions like sulfide, phosphate, and hydroxide, it predominantly remains in the solid phase, allowing iron to be transferred to downstream units. For instance, it reduced dissolved sulfide concentrations by 32.2±3.3% (at 0.58 ±0.5 mg S/mg Fe, or 1.0 mol Fe/mol S) in sewer reactors, decreased phosphate concentrations by 38.3±3.2% (at 0.37±0.04 mg P/mg Fe, or 1.5 mol Fe/mol P) in sequencing batch reactors, and lowered dissolved sulfide concentrations by 72.0±4.2% (18.9±2.4 mg S/L) in the anaerobic sludge digester, compared to the control that received no chemical dosing. The iron-rich sludge in the $FeCO_3$-dosing system also exhibited better sludge settleability and digested sludge dewaterability, with improvements of 33.9 ± 5.5% and 15.9 ± 2.0%, respectively. Additionally, dosing $FeCO_3$ in sewers provides additional alkalinity, which is favourable for sulfide precipitation in sewers and the downstream nitrification process. Overall, the long-term results demonstrate the practical feasibility of $FeCO_3$ application in integrated urban wastewater systems, delivering environmentally friendly solutions for chemical production and biogas upgrading.

Presenter's Biography

Dr Min Zheng is an Associate Professor at UNSW. Since establishing his academic career in Australia in 2019, he has been dedicated to advancing the research group Green Environmental Technologies for Sustainability (GetSustain). This group focuses on developing innovative solutions to critical issues in the water industry, emphasising biochemical processes for net-zero emissions, waste recycling, and urban water infrastructure. His significant contributions to the field are reflected in his extensive publication and grant records, as well as recognition from his peers.

Revolutionizing Multifunctional Subaquatic Apparatus via Advanced Structural Engineering of Nanocarbon Materials

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A paradigm shift is underway in underwater technology, driven by advanced nanocarbon structural engineering. The age-old challenge of effective underwater adhesion is conquered with a novel approach inspired by the water transportation in plants that deftly channels residual liquid away from the adhesion interface, ensuring robust locking and substrate sealing. Crafted from low-dimensional materials like CNT, Graphene, and MXene, this adhesive material features a high-aspect-ratio vertical channel for swift water transport and multiple mesopores that enhance liquid storage efficiency. A remarkable adhesive strength of 216.5 ± 5.5 kPa is achieved, surpassing the 100 kPa benchmark for underwater adhesives. Cycling endurance soars to an unprecedented 100,000 cycles, while a rapid 1.5-second adhesion cycle time sets a new standard. Mechanistic insights unveil the synergy between submicron vertical channels and surface cup area fractions, amplifying adhesion prowess. Shifting focus to pressure sensors, a groundbreaking self-adhesive sensor emerges, combining aligned and nonaligned carbon nanotube components. It detects pressures as low as 18 mPa with remarkable linearity, while the nonaligned component ensures effective underwater adhesion and secure fixation. This sensor extends the detectable pressure range by four orders of magnitude, akin to air applications. Fusing artificial neural networks with the sensor achieves flawless underwater target recognition. This transformative narrative marks the dawn of a new era in multifunctional subaquatic technology, driven by ingenious nanocarbon structural engineering [1,2,3].

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Presenter's Biography

Ming Xu is a Full Professor at the School of Materials Science and Engineering, Huazhong University of Science and Technology. She was selected for the National Overseas High-Level Talent Youth Program (Priority Support) and the Hubei Province Outstanding Talent Program. Her primary research focuses on the fabrication and application development of nanocarbon macroassemblies. Her research approach is driven by practical application needs and performance optimization, with the controllable synthesis as the core. Her work addresses key scientific challenges associated with the performance of these materials in extreme environments and aims to achieve transformative improvements in their functional properties. She has published over 60 papers in high-impact journals, including Science (2 papers), Nature sister journals (3 papers), and Cell family journals (2 papers). She holds 25 authorized patents and has achieved a series of groundbreaking innovations. These include a super rubber capable of stable performance in a temperature range of -196°C to 1000°C, a carbon-based adhesive functional between -196°C and 1033°C, a high-sensitivity carbon-based sensor for marine environments, and high-performance carbon-based energy storage devices operating at -60 °C to -100°C. Notably, the super rubber extends the operating temperature range of existing rubber materials by thousands of degrees, earning her the prestigious Iijima Award in 2011, making her the youngest recipient of this honor. Additionally, her development of a self-powered wave monitoring and tsunami early warning device has improved the accuracy of underwater pressure detection by an order of magnitude, winning the Gold Award with Special Commendation from the Jury at the 2019 Geneva International Exhibition of Inventions.

Structural designs of graphene fluoride for improved thermoconductive polymer composites

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The demand for effective thermal management in the electronics, aerospace, and automotive sectors is driving the search for materials with exceptional thermal conductivity.[1] Graphene fluoride (GF), a variant of graphene chemically modified with fluorine atoms covalently bonded to its carbon lattice, offers a promising approach for enhancing the thermal properties of polymer composites.[2] This research fabricated various structural architectures of graphene fluoride and investigated the incorporation of structured graphene fluoride into polymer matrices to create thermoconductive composites with enhanced thermal performance and mechanical strength.[3] Our results show a marked improvement in thermal conductivity with the addition of graphene fluoride. This enhancement is attributed to the efficient phonon transport provided by the two-dimensional structure of graphene fluoride and the improved interfacial thermal resistance. The combination of increased thermal conductivity and excellent mechanical and thermal stability makes graphene fluoride-based composites a strong contender for next-generation thermal management solutions in high-performance applications.

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Presenter's Biography

Dr. Minh Canh Vu currently joined Precision Mechatronics Lab as a Research Associate at the University of Newcastle (06/2024). He obtained Ph.D. in Polymer Science and Engineering from Korea National University of Transportation, where his research focused on the application of graphene fluoride nanosheets for the fabrication of thermoconductive polymer composites. Dr. Vu worked as a Postdoctoral Researcher at the University of Chicago (2021-2024), where he has made significant contributions to the characterization of molten salt electrolytes for lithium metal and dual-ion batteries. His extensive research portfolio encompasses energy storage solutions, thermal management materials, electromagnetic interference (EMI) shielding, and additive manufacturing.

Dual-carbon battery with a nonflammable solventless electrolyte: A safe, low-cost, eco-environmental energy storage

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The intermittent and diffuse nature of renewable energy sources necessitates efficient energy storage and conversion infrastructure. Lithium-ion batteries (LIBs) are widely used in portable electronics, electric vehicles, and grid storage due to their high energy density and cycling stability. However, the limited availability of lithium, nickel, and cobalt, alongside recycling challenges, underscores the need for cost-effective alternatives with superior performance. Dual-carbon batteries (DIBs), involving the intercalations of cations and anions to carbon-based electrodes, are emerging as a promising energy storage solution, characterized by cost-effectiveness, high voltage, and environmental friendliness. Conventional electrolytes in DIBs, based on carbonate solvents, suffer from oxidative instability, leading to decomposition and restricted cycling stability under high voltage, and the usage of volatile and flammable solvents raise the safety issues. This work introduces a dual-carbon battery with nonflammable solventless electrolyte, representing a significant leap forward in the quest for sustainable, intrinsically safe, and high-performance energy storage systems.

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Nanocarbon's Innovation toward Carbon Circular Economy

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The Circular Carbon Economy (CCE) emerges as a pivotal paradigm in carbon management, offering an innovative approach to evolving our understanding and utilization of carbon. The CCE framework holds the potential to guide us towards a more inclusive, resilient, and ultimately sustainable energy system, aiming for carbon neutrality or net-zero emissions. Crucially, CCE emphasizes that hydrocarbons and carbon materials can maintain their significance in this transition. This perspective underscores the pivotal role of carbon management in shaping a sustainable future and provides a vital roadmap for carbon circular research.

From the perspective defined by the CCE, traditional carbon materials as well as emerging nanocarbons can play crucial roles in this field. Taking carbon nanotubes (CNTs) as a representative nanocarbon material, in the catalytic chemical vapor deposition (CCVD) process 1 , carbon fixation can be achieved through the utilization of biogas, making it an effective method for CNT and hydrogen production as an environmentally friendly process. CNTs thus manufactured can be effectively utilized in lithium-ion batteries(LIB), contributing to CO2 reduction as electric vehicle batteries and storage in LIB of the power generated from renewable energy, which are expected to play a significant role in the future.In the construction of the global renewable energy power grid, CNT conductor wires are expected to be applied to replace copper cables, addressing concerns of resource depletion. Furthermore, carbon nanotubes will also contribute to various water treatments using reverse osmosis membranes and green hydrogen production by PEM. Such challange for nanocarbons innovation can contribute to CCE

Here, focusing mainly on nanocarbons, particularly on carbon nanotubes, their expected contribution to CCE will be shown and discussed.

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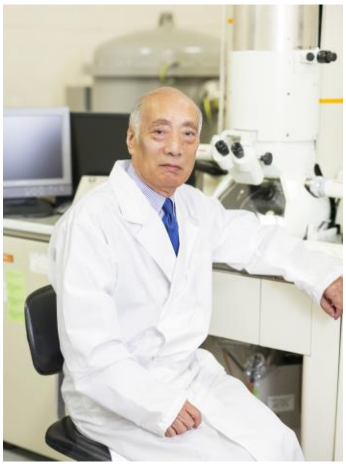
M.Endo, Distinguished Prof. of Shinshu University,has been studying on basic science and applications of carbon materials, focusing on nanocarbons.



Tailored Production of Bio-based Hard Carbon from Agricultural Biomass for Sodium-ion Battery Anode Application

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Abstract: Sodium-ion batteries (SIBs) hold considerable commercial promise as complementary energy storage technology to lithium-ion batteries (LIBs), which rely on more expensive lithium products. However, the commercialization of SIBs is hindered by their comparatively lower ion storage capacities, lower initial coulombic efficiencies (ICE) and lower rate capabilities, leading to lower energy densities than LIBs. Hence, developing advanced anode materials is crucial for enhancing the electrochemical performance of SIBs. Hard carbon (HC) has emerged as the most prospective high-performance anode material for SIB applications. Another significant barrier to the commercialization of SIBs is the cost of anode materials. While sodium compounds are more affordable than lithium compounds, the anode materials for SIBs are significantly more expensive. Hence, using bio-based precursors such as lignin as the precursor for HC can help mitigate these costs, as it is a low-cost substrate with a relatively high carbon content. The aromatic regions, crosslinking and functional groups inherent to stable lignin are advantageous for synthesizing HC over other precursors like sugars and carbohydrates. In this regard, agricultural biomass was pretreated using different solvents to obtain modified lignin. Extracted lignin was used as the precursor to produce HC and fabricate high-performance anode material for SIBs. The fundamental understanding of property relationships between lignins and HCs is crucial for developing biomass-based anode material. This approach promises to contribute to producing cost-effective, sustainable SIBs for energy storage applications.

Nethmi Kulanika Dayarathne completed her bachelor’s degree (hons) in Chemistry in 2021 from University of Colombo, Sri Lanka. After completing her bachelor’s degree, she worked as Teaching Assistant in the Department of Chemistry, University of Colombo, Sri Lanka. In 2022, she joined Cnetre fro Agriculture and the Bioeconomy at Queensland University of Technology, Australia to pursue her PhD studies. She currently woking on the development of high performance anode materials from agricultural waste for alternative sodium-ion battery application.

Nano-structured porous carbon materials for enabling ultrafast gas hydrate formation for energy storage and carbon sequestration

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Water and gas (hydrogen, methane, etc.) don't mix. Yet, one can use water as a means for gas storage. This paradox presents a fascinating field of science and technology - gas hydrate [1]. Gas hydrate is an extraordinary form of matter where hydrophobic gas, which is nearly insoluble in liquid water, is encapsulated massively in the cavities of a solid structure of water. Hence, gas hydrate is a water-based structure similar to ice, but it is distinct from ice by containing large fractions of gas. For example, the mass fraction of methane and hydrogen in their gas hydrate is up to 13.3 wt.% and 4.5 wt.%, respectively.

Massive inclusion of fuel gas in solid water offers a rare opportunity for using gas hydrate as a means of sustainable gas storage, especially hydrogen storage [2], taking the advantage of water as the cheapest, safest and most sustainable raw material. However, the poor mixing between the gas and liquid water presents a grand challenge for scaling up toward applications. Nano-structured surface-engineered porous carbon materials as "nanoreactors" allow to overcome the intrinsic bottleneck related to the poor mixing between the gas and liquid water (Figure 1), which in turn enables rapid gas hydrate formation for novel energy storage (for fuel gas) and carbon sequestration (for carbon dioxide).

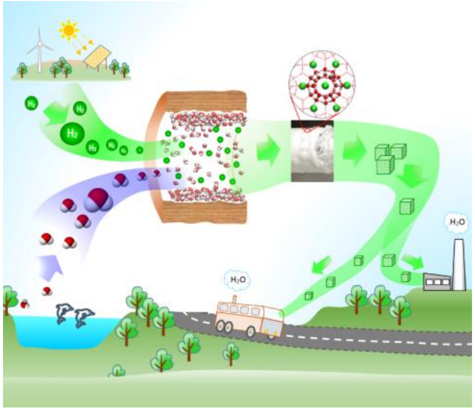

Fig. 1. Nano-structured materials as "nanoreactors" to enable novel fuel gas storage using gas hydrate [1,3].

I will present this novel method for energy storage and carbon dioxide sequestration using gas hydrate as a gas-bearing water-based structure. I highlight the central role of nano-structured surface-engineered porous carbon materials for boosting the kinetics of gas hydrate formation for enabling the above-mentioned applications in the low-emission future.

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Presenter's Biography

Ngoc N. Nguyen is an ARC DECRA Fellow in The University of Queensland (UQ). He obtained a PhD in Chemical Engineering (UQ) in 2018. Then, he was awarded an Alexander von Humboldt Fellowship and worked for Max Planck Institute for Polymer Research in Germany (2019 – 2021). He also worked as a visiting scholar at Pacific Northwest National Laboratory in USA (2015) and a lecturer at Hanoi University of Science and Technology in Vietnam (2018). His research focuses on interfacial 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.

Engineered Nanocatalyst for Biomass Electro-Conversion Reactions: Sustainable Chemistry Using Renewable Electrons

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The adaptation of electrocatalysis to biomass conversion reactions is showcasing its prowess in the sustainable chemistry landscape. With the ever-dropping cost of renewable electrons, electrocatalysis has potential to supplant a portion of traditional thermochemical routes, often with enhanced reaction selectivity. Common approaches adapt engineering constructs and scientific principles from water electrolysis reactions, mostly focusing on biomass electrooxidation at the anode to liberate free protons for H_2 generation at the cathode. In principle, biomass oxidation occurs at lower overpotentials than the oxygen evolution reaction (OER), providing added value through the production of commodity hydrocarbons over O_2 with a decreased energy input. While current efforts to date are encouraging, the scope of efforts reported today are often limited to simple alcohol and aldehyde oxidation reactions and often implement established catalytic materials for OER. Such approaches miss out on opportunities for coupling chemistries, reductive biomass processes, and subsequent catalyst engineering that is needed to fully electrify biomass conversion processes. In addition, waste water treatment, often involving the removal of biomass from water, is another application area where such reactions can be used to generate sustainable chemistry from waste.

In this contribution, our group's work on examining a range of biomass electrocatalytic reactions will be summarized, with an emphasis placed on engineering new catalytic materials that pivot away from traditional OER catalysts. Materials exhibiting low OER reactivity are used here, which conversely exhibit excellent selectivity toward the hydrocarbon processing, even at higher overpotentials need to maintain high reaction rates. To establish structure/property relationships, in-situ synchrotron radiation characterization techniques are employed to elucidate active site structure during electrocatalytic reactions with atomic-scale resolution. The summation of these efforts provides pathways forward for future electrocatalytic processing for biomass, providing routes forward sustainable chemistry using renewable electricity.

Presenter's Biography

Nicholas Bedford is an academic the School of Chemical Engineering and chief investigator in the Centre of Excellence in Carbon Science and Innovation at the University of New South Wales, Australia, and holds an affliate appointment at Colorado School of Mines. His research interests broadly revolve around solving the structure-property relationship question in nanoscale materials, where his group uses advanced synchrotron characterization and modeling technique to reveal atomic-scale structure. His group applies these approaches in a range of application spaces, including electrocatalysis, environmental chemistry, advanced ceramic materials, and biosensors.

EPR Applied to Materials Science

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Electron Paramagnetic Resonance (EPR) spectroscopy is experiencing a renaissance, with new applications allowing unique physical characterization of many different types of matter, from well-defined to intrinsically disordered small and large molecules (e.g. peptides and proteins) as well as high end materials e.g. zeolites to battery electrodes (1). The high contrast of EPR allows the target component (unpaired electrons) to be viewed in isolation from a large background, making it complementary to more universally employed characterization techniques such as NMR and crystallography.

The EPR facility based at the ANU represent part of Australia's core EPR infrastructure, hosting Australia's only High Field EPR Instrument (LE170100023 – Australian High Field Facility). This national facility is routinely accessed by researchers across Australia and New Zealand and allows multi-frequency EPR measurements over a large frequency range (9 to 100 GHz), in both continuous wave (CW) and pulse operation, with broad applications across Medicine, Biology, Chemistry and Materials Science. This facility is being constantly ugraded to maintain Australia's position at the forefront of EPR research.

In my talk I provide a range of examples of the use of EPR in current research (2-3). I will focus on examples from materials chemistry including: 2D materials, photocatalysts, battery electrodes and functional materials, drawn from recent collaborative projects. If time permits, I will also show recent methodological developments of my group towards locating and characterizing magnetic nuclei both adjacent to and distant (up to 3 nm) from EPR visible paramagnetic sites (4-5). We've used such methods in biocatalysis and in structural biology, specifically for locating substrate/drug binding sites, but these are general methods and are readily translatable to materials systems.

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Presenter’s Biography

Prof. Nick Cox is an spectroscopist based at the Australian National University. His research focuses on method development in magnetic resonance spectroscopy, with broad applications in Medicine, Biology, Chemistry and Materials Science. He established and now manages Australia’s only high-field (W-aband) Electron Paramagnetic Resonance (EPR) instrument (LE170100023) - existing Australian facilities operate at a magnetic field strength three-fold lower. This facility aims to be a national resource, open to researchers across the Asia-Pacific. Since 2020, the facility has contributed to projects based at: RMIT, Macquarie University, University of Western Australia, University of NSW, Monash University, University of Tasmania, University of Melbourne, Otago University (New Zealand), CSIRO and others.

Insights into Atomic Level π-Electron Modulations in Supramolecular Carbon Nitride Nanoarchitectonics for Sustainable Green Hydrogen Production

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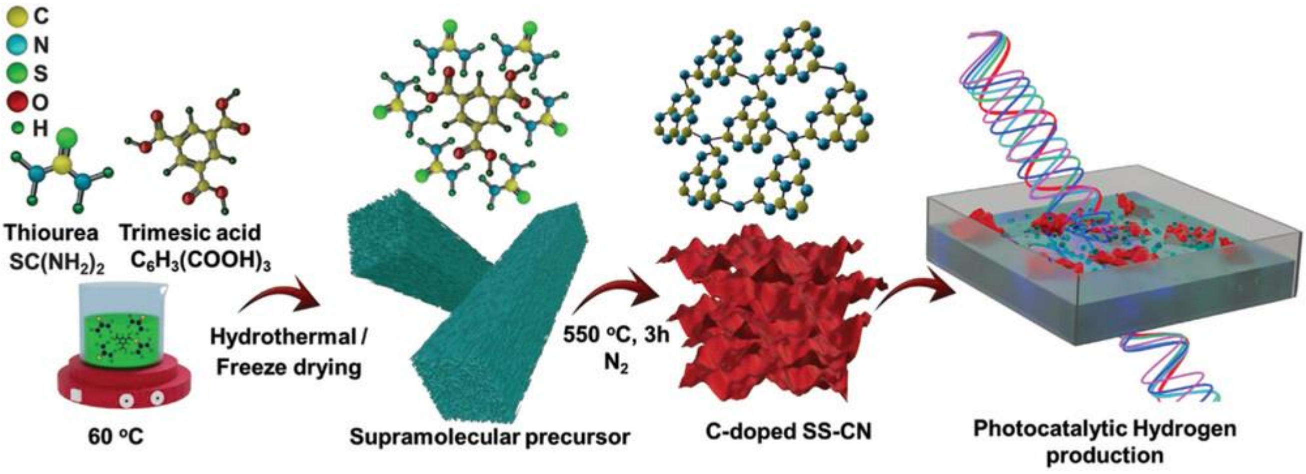
https://doi.org/10.1002/aenm.202400686

Carbon nitrides, as metal-free semiconducting materials, possess unique molecular structures and semiconducting properties, making them promising photocatalysts for sustainable hydrogen production. However, their potential is limited by drawbacks such as fast charge-carrier recombination and low charge transfer efficiency, mainly due to their amorphous and poorly conducting structure. These issues remain significant challenges for advancing photocatalytic water splitting. This study presents a supramolecular approach that couples thiourea and trimesic acid to design highly efficient C-doped carbon nitride photocatalysts, where the π-electron density is precisely controlled. The resulting C-doped carbon nitride shows finely tuned band positions, reduced electron-hole recombination, and enhanced conductivity, leading to significantly improved hydrogen generation through photocatalytic water splitting under solar-simulated light. Advanced techniques, including X-ray photoelectron spectroscopy, near-edge X-ray absorption fine structure spectroscopy, and electron paramagnetic resonance spectroscopy, were used to characterize the position and distribution of C-doping in the carbon nitride framework. Additionally, first-principles studies of the electronic structure and doping energetics were conducted. The remarkable increase in photocatalytic hydrogen production using the developed C-doped carbon nitride brings us a step closer to realizing a green hydrogen economy.



Covalent Thin Films for Energy Applications and Beyond

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The interest behind carbon-based materials is recently rising and structures with specifically designed properties and chemical features have widened the application opportunities of this materials' class. Exemplarily, the introduction of lightweight heteroatoms, such as boron, nitrogen, and oxygen into a pool of sp^2-bonded carbon expands the spectrum of possibilities and enables tailoring the electronic and optical properties of these materials.[1] Furthermore, the ability to control their shape in the form of two-dimensional coatings with nanometer-sized thickness, opens up a wide range of opportunities for their application in energy storage and conversion, among others.[2,3]

At the higher end of nitrogen doping, semiconductors of the family of carbon nitrides, a class of covalent materials with ideal formula C_3N_4, have recently attracted much attention especially in photocatalysis with visible light. However, up to now, their application as thin films has been hindered due to the low homogeneity of the coatings available. Here, we developed a method based on chemical vapor deposition (CVD) that enables to deposit carbon nitride thin films with tuneable thickness over large substrates, regardless their shape.[4] This method paved the way for the application of these thin films in energy storage and photocatalysis, e.g. increasing the plateau capacity of carbonaceous electrodes in sodium-ion batteries,[5] enabling the development of batch and microfluidic reactors,[6] and innovative methods for the in-operando studies of reaction mechanisms.

The utilization of covalent semiconductor thin films, such as carbon nitrides, in energy storage and conversion is still in its infancy, however, it sets the premises for the development of significant improvements in these fields and beyond, such as in optics and surface science.

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Paolo Giusto is a Group Leader at the Max Planck Institute of Colloids and Interfaces, Colloid Chemistry Department, in Potsdam (Germany), where he currently leads an international research team. His research focuses on the synthesis of covalent materials and thin films with specific chemical, electronic, and structural properties for application in energy storage and conversion. He is currently involved in several national and international projects for the application of covalent thin films in energy storage and conversion. In his free time, he enjoys playing football and cooking.

Chemical and physical sensing with low-dimensional nanostructures: the disruptive power of supramolecular chemistry

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Low-dimensional nanostructures exhibit a high surface-to-volume ratio which makes their physical and chemical properties highly sensitive to environmental changes. While such a unique sensitivity can be used for the realization of chemical sensors, the unspecific nature of the interactions with the environment drastically limits the selectivity in the sensing events. On the other hand, supramolecular (multi)functional materials are held together by reversible and highly specific interactions between suitably designed building blocks. The use of non-covalent interactions to build sophisticated supramolecular architectures makes it possible to transduce the modifications of their environment into precise modulation of their self-assembly behaviour. The changes of properties upon small environmental variations can be enhanced or amplified by integrating the assemblies into working devices.

Low-dimensional nanostructures chemically functionalized with supramolecular receptors of the analyte of interest can therefore be the key active components for the development of the next generation of sensors exhibiting detection limits down to sub-ppb level combined with fast response speed and unprecedented selectivity. Such a strategy can enable the future fabrication of ultrasensitive and ultraselective sensors for food safety, environmental and biohealth monitoring, as well as for chemical- and biodefense, thus providing a decisive contribution to the improvement of people's quality of life.

In my lecture, I will review our recent endeavour on the tailoring of low-dimensional nanostructures chemically functionalized with the receptors of the target analytes and on the use of these hybrid assemblies to fabricate chemical sensors with an electrical or optical read out, which combine high sensitivity, selectivity, response time and reversibility. In particular, we will focus on chemically functionalized 0D (network of metallic nanoparticles), 1D (supramolecular fibers) and 2D (graphene and other layered materials) for humidity, heavy metal and polyaromatic sensing as well as for the generation of pressure sensors for the diagnosis of cardiovascular diseases.

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Presenter's Biography

Paolo Samorì is Distinguished Professor at the University of Strasbourg and Emeritus Director of the Institut de Science et d'Ingénierie Supramoléculaires (ISIS). He is Member of the Académie des technologies, Member of ACATECH, Foreign Member of the Royal Flemish Academy of Belgium for Science and the Arts (KVAB), Fellow of the Royal Society of Chemistry (FRSC), Fellow of the European Academy of Sciences (EURASC), Member of the Academia Europaea, Fellow of the Materials Research Society (MRS) and Senior Member of the Institut Universitaire de France (IUF). He published 460+ papers on nanochemistry, supramolecular sciences and materials chemistry with a specific focus on two-dimensional materials and functional organic/polymeric nanomaterials for optoelectronics, energy storage and sensing.

Phase stabilization strategies for efficient perovskite solar cells

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The recent decade has witnessed the rapid increase in the power conversion efficiency of metal halide perovskite solar cells from 3.8% to certified 26.7%. Despite their success in achieving intriguing photovoltaic performance, the inferior phase stability of PSCs against external stimuli (e.g. moisture, oxygen, UV light) remains a critical hurdle for their further large-scale applications. Herein, we introduced innovative strategies, including interfacial engineering,[1-3] surface ligand decoration,[4] redox shuttle antioxidant,[5] and material composition,[6] to stabilize the photoactive phase and simultaneously passivate surface defects of perovskites for optoelectronic applications. By rational design on interfacial and surface engineering, the fabricated lead-based or tin-lead-mixed perovskite solar cells showed improved power conversion efficiency and exceptional durability under operational conditions. Besides, the synthesized perovskite-metal organic framework composites showed excellent photoluminescence stability against water immersion for 10,000 hours, which can serve as a desirable encapsulation technique for perovskite optoelectronics in the future.

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Biography

Dr. Peng Chen is an ARC DECRA Fellow in Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland. In 2020, he got his PhD degree from School of Chemical Engineering at UQ under the supervision of Prof. Lianzhou Wang, before moving to AIBN to work as an Australian Centre for Advanced Photovoltaics (ACAP) Research Fellow during 2020-2022, and started his ARC DECRA Fellowship in 2023.

Temporal, Spatial and Thermal Dynamics of Intracellular Organelles Revealed by Biophysical Nanotools and Advanced Imaging

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The intracellular metabolism of organelles, like lysosomes and mitochondria, is highly coordinated spatiotemporally and functionally [1, 2]. The activities of lysosomal enzymes significantly rely on the cytoplasmic temperature, and heat is constantly released by mitochondria as the byproduct of adenosine triphosphate (ATP) generation during active metabolism. Here, we developed temperature-sensitive LysoDots and MitoDots to monitor the in situ thermal dynamics of lysosomes and mitochondria [3, 4]. The design is based on upconversion nanoparticles (UCNPs) with high-density surface modifications to achieve the exceptionally high sensitivity of 2.7% K21 and low uncertainty of 0.8 K for nanothermometry to be used in living cells. We show the measurement is independent of the ion concentrations and pH values. With Ca2+ ion shock, the temperatures of both lysosomes and mitochondria increased by ∼2 to 4 °C. Intriguingly, with chloro- quine (CQ) treatment, the lysosomal temperature was observed to decrease by up to ∼3 °C, while mitochondria remained relatively stable. Lastly, with oxidative phosphorylation inhibitor treatment, we observed an ∼3 to 7 °C temperature increase and a thermal transition from mitochondria to lysosomes. These observations indicate different metabolic pathways and thermal transitions between lysosomes and mitochondria inside HeLa cells. The nanothermometry probes provide a powerful tool for multi-modality functional imaging of subcellular organelles and interactions with high spatial, temporal, and thermal dynamics resolutions.

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Presenter's Biography

Dr QIAN (Peter) SU is now an Australian NHMRC EL1 Fellow and a Senior Lecturer at the University of Technology Sydney. He received PhD in Biophysics from Peking University, China with a joint training at Harvard University, US (visiting scholar 2012). His research program named “Quantitative Imaging at Nanoscale with SUper-resolution (QIAN SU)” bridges applied biomedical engineering with fundamental sciences and medical requests, which brings new insights to mechanistic questions addressed at the single-molecule level by advanced microscopy.

Designing and Probing Metal Based Electrocatalysts for Energy Conversion Applications

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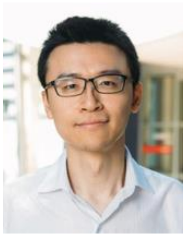
In this presentation, we explore the role of heterogeneous electrochemical processes at electrode interfaces in converting, storing, and utilizing clean energy. The development of high-performance inorganic electrocatalysts capable of sustaining electrochemical turnover under operando conditions remains a significant challenge. It is essential to understand the structural, crystal, and electronic properties of these activated electrocatalysts during operation to investigate their mechanisms and assess their performance. We will discuss the application of in-situ characterizations such as X-ray Absorption Spectroscopy (XAS), X-ray Diffraction (XRD), Raman spectroscopy etc., to confirm the presence of metal based catalysts (TM = Mn, Fe, Co, Ni, Cu, Ru, Bi, Ag) as electrocatalysts for the Oxygen Reduction Reaction (ORR), Oxygen Evolution Reaction (OER), Hydrogen Evolution Reaction (HER) and Carbon Dioxide Reduction Reaction (CO2RR) and examine their electrochemical transformation from precursor states. The observed enhancements in electrocatalytic activities are attributed to the electronic modulation of the transition metals by the substrates or the unique chemical environments within the nanoscopic structures.

Presenter's 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, an Australian Research Council Discovery Early Career Researcher Award in 2017 and Australian Research Council Future Fellowship in 2024. He is currently an Associate Professor in Centre for Catalysis and Clean Energy and the School of Environment and Science, Griffith University, focusing on synthesis, in situ characterizations, and electrocatalytic applications of nanostructured catalysts in energy conversion and storage devices.

Understanding and Designing Additives for Durable Aqueous Zinc Batteries

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Aqueous zinc-ion batteries are regarded as promising energy storage systems for next-generation residential and commercial storage due to their high theoretical energy density, low cost and safety. However, their practical development is hindered by zinc anode corrosion and dendrite formation, thus negatively affecting durability and device functionality. Therefore, the development of electrolyte systems, by employing organic additive molecules for example, that enable durable zinc anodes is an interesting solution to push the zinc-ion batteries toward commercialization. In this talk, I will focus on the role of such additives in limiting zinc corrosion and thus, improving the lifetime of zinc anodes. I will also discuss a roadmap for designing and screening new additives based on the understanding we derived.

Presenter's Biography

Dr. Priyank V. Kumar is a Scientia Senior Lecturer in chemical engineering at UNSW Sydney. He was awarded his PhD in materials science from MIT, USA in 2015, after which he was a postdoctoral fellow at ETH Zurich until 2019. His research group is interested in understanding and designing nanomaterials using theory, computation and data-driven/machine-learning methods by collaborating with experimentalists. The group's focus is on applications including catalytic systems, batteries, and functional polymers.

Fabrication of Carbon/Polymer Composites via Photopolymerization

X. Peng [1] *and P. Xiao* [2]

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Composite materials consisting of functional polymers and carbon materials have been attracting considerable attention owing to their remarkable properties and multi-functionalities. Despite their enormous potential applications, some problems still need to be solved in the existing synthetic methodologies, including the incompatibility between organic polymers and inorganic materials, the long reaction times, agglomeration, and high cost of the precursors. In this presentation, a novel one-step approach for in situ fabrication of polymer/carbon composite nanomaterials by the photopolymerisation technology,[1-5] which is expected to solve the aforementioned problems encountered in existing synthetic methodologies, will be demonstrated. Specifically, this talk will present our developed long-wavelength sensitive photoinitiators for photopolymerisation of various monomers/oligomers under visible light irradiation. These will be used to produce polymer/carbon composite materials that can thus be fabricated through a one-step polymerisation process.

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Presenter's Biography

Pu Xiao worked as a postdoctoral fellow at the Fachhochschule Nordwestschweiz (Switzerland) and the CNRS (France) after obtaining his PhD. Following this, he joined the University of New South Wales as a Lecturer before being appointed Senior Lecturer and then promoted to Associate Professor at the Australian National University. He moved to Chinese Academy of Sciences as a Professor. His research interests include green composite biomaterials, photophysical chemistry, photopolymerization technology, 3D printing, and light-induced responses of materials.

The Promotion of Emerging Carbon Energy Materials for Next-Generation Batteries through Lithium Bond Chemistry

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As one of the most important applications of the element, Li batteries afford emerging opportunities for the exploration of Li bond chemistry. In this talk, the historical development and concept of the Li bond are reviewed, in addition to the application of Li bonds in lithium-sulfur batteries. The Li bond was described in the context of Li batteries, including discussions of emerging carbon materials for sulfur cathodes, liquid electrolytes, and Li metal anodes. Such discourse on the chemistry of the Li bond can provide fruitful insight into the fundamental interactions within lithium-sulfur batteries and thus deliver a deeper understanding of their working mechanism.

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Presenter's Biography

Prof. Qiang Zhang is a full professor at Tsinghua University. He held the Newton Advanced Fellowship from Royal Society, UK and the National Science Fund for Distinguished Young Scholars. He is selected as highly cited researchers at 2017-2023 by Clarivate Analytics. His current research interests are advanced energy materials, including dendrite-free lithium metal anode, lithium sulfur batteries, and electrocatalysis, especially the structure design and full demonstration of advanced energy materials in working devices. His h-index is 166 now. He is the Editor-in-Chief of EES Batteries, Advisor Editor of Angew. Chem., Associate Editor of J Energy Chem. He is sitting on the advisory board of Joule, Chem Soc Rev, Matter, Adv Funct Mater, ChemSusChem, J Mater Chem A, Chem Commun, Energy & Fuels, and so on. He is the deputy head of the expert group on energy storage and smart grid of the national key research and development plan. He has won the first prize of Natural Science of the Ministry of Education, the first prize of Fundamental Science of the Chemical Engineering Society.

Carbon Dot-Based Hybrid Quantum Materials for Photocatalysis

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Quantum materials are materials that exhibit non-classical properties, and are governed by quantum excitations and quasi-particles such as electrons, magnons, excitons, and polaritons, among others. Heterostructures of quantum materials are particularly interesting, because they provide manipulation routes to either trap or guide the quasi-particles and alter the energy states. Colloidal synthesis using Ligand mediated surface engineering is a powerful approach to synthesize quantum dots, rods and platelets. Its versatility and readiness for upscaling has earned it the 2023 Nobel Prize. In this talk, we present a colloidal synthesis method to grow high-quality carbon quantum dots (CQDs) on ZnSe nanoplatelets (NPLs), i.e., metal chalcogenide quantum wells. [1, 2] The resultant organic-inorganic hybrid nanoparticles, CQD-NPLs, are able to perform methanol dehydrogenation with the occurrence of α-C-H splitting and C-C coupling. The novel CQD-based organic-inorganic heterostructure quantum material is poised to enable the discovery of a host of new nano-hybrid photocatalysts with full tunability of the band structure, charge transfer, and divergent surface chemistry for guiding photoredox pathways and accelerating reaction rates.

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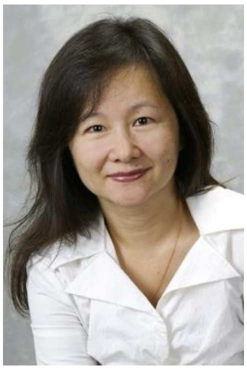

Dr. Qin Li is a Professor of Environmental Engineering at Griffith University. She obtained her PhD in Chemical Engineering from the University of Queensland (2002) and BEng (1994) and MEng degrees (1997) from Zhejiang University. Dr. Li conducts research on functional materials, catalysis and applied nanotechnology to provide solutions for renewable energy, environmental monitoring, water purification, and waste reformation. With two edited books, 6 book chapters, over 140 journal papers and 4 international patents with an *h*-index of 53 (Google Scholar), Qin is ranked in the top 2% of researchers across all discplines in the world by Standardford Analysis. Qin is a former Marie Curie Fellow at the Max Planck Institute for Polymer Research, winner of Curtin Innovation Award 2009, and the finalist of Women in Technology Research Award in 2015 and 2020. Qin is also the Co-Founding Chair of the Green and Sustainable Chemistry & Engineering National Interest Group at RACI, and advocates for Innovating Sustainably.

Probing the active site of carbon-based catalysts by EC-STM

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Active sites in catalysts play key roles in determining their efficiency and reaction pathways in electrochemical reactions. Probe and confirm the active sites in catalyst is important to design and synthesize the high-efficient catalysts for specific applications. Electrochemical scanning tunneling microscopy (EC-STM) offers a direct, atomic-scale method to probe these active sites, enabling real-time observation of surface structures and electronic properties under operational conditions. In my study, I utilize EC-STM to explore the active sites of carbon-based catalysts, revealing the key structure-activity relationships. Further, it can provide critical insights into the mechanism of electrochemical processes, advancing the rational design of carbon-based materials for various applications.

Presenter's Biography

Dr Qingfeng Zhai is currently an ARC DECRA Fellow at the Australia Carbon Materials Centre (A-CMC), School of Chemical Engineering, University of New South Wales (UNSW Sydney). Dr Zhai received his PhD degree from Changchun Institute of Applied Chemistry (CIAC), Chinese Academy of Sciences (Changchun, China) in 2018, with his research focusing on the fabrication of various high-efficiency electrochemical sensors. From 2018 to 2020, Dr Zhai worked as a Postdoctoral Research Associate at Monash University, developing highly flexible energy storage and sensing devices for wearable applications. After that, Dr Zhai moved to UNSW Sydney, working under the supervision of Prof. Liming Dai as a senior Postdoctoral Research fellow. Currently, his research focuses on carbon-based materials for electrocatalysis and sensing applications. This includes using the advanced in-situ characterization technique, such as electrochemical scanning tunneling microscope (EC-STM), for the catalytic mechanism study from the atomic scale, as well as screening or developing highly efficient carbon catalysts for diverse applications, including energy conversion and green chemistry.

Fine tuning the oxygen electroreduction under different scales for H_2O_2 synthesis

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Electrochemical oxygen reduction reaction (ORR) through a $2e^-$ pathway provides a feasible approach for the electrosynthesis of H_2O_2 in an eco-friendly manner. However, the practical implementation of such method is severely restricted by the poor apparent electrocatalytic performance on the ORR cathode. To resolve this issue, we fine engineered the ORR active moieties under atomic scale, such as cobalt single atoms and polymerized boron-nitrogen-carbon composites, through rationally modifying their coordination structures and surface oxygen environment, aiming to optimize the adsorption state of ORR intermediates and suppress the other side reactions on the catalysts.[1,2] As such, an improved intrinsic 2e- ORR performance was obtained, giving a high H_2O_2 selectivity in a wide range of pH environment. In addition to a superior intrinsic activity, an efficient mass transfer is also of significant importance for securing an improved apparent H_2O_2 yield. In this regard, we further designed and developed a three-dimensional porous electrode structure anchored with abundant highly active moieties as obtained above. Due to the formation of abundant liquid/gas/catalysts three-phase interfaces and a rapid mass/charge transfer, a high apparent activity and H_2O_2 productivity were exhibited during ORR in a practical O_2 electrolyzer (Fig. 1).[3]

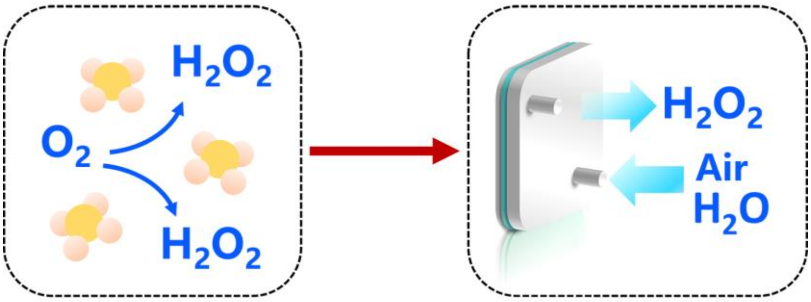

Fig. 1 Schematic illustration of H_2O_2 electrosynthesis via ORR under different scales: from active site engineering to device design for an improved apparent H_2O_2 productivity.

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Presenter's Biography

Qingran Zhang:

Dr. Qingran Zhang is currently an Associate Professor and Distinguished Research Fellow at the School of Environmental Science and Engineering, Tongji University, Shanghai, China. He received his Ph.D. degree in Chemical Engineering at the University of New South Wales (UNSW) in 2020 under the supervision of Prof. Rose Amal. His research interest focuses mainly on the design of cost-effective and active catalysts for electrochemical energy conversion systems (including water splitting for green hydrogen production, oxygen reduction reaction for hydrogen peroxide synthesis and other selective electrochemical processes for resource recovery/environmental remediations) and the device development for efficient utilization of renewables.

White Graphene: Thickness-Related Properties and Applications

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Because boron nitride nanosheets (BNNSs) are structurally similar to and isoelectronic with graphene, they are often referred to as "white graphene". BNNSs not only inherit most of the outstanding properties of hexagonal boron nitride (*h*-BN), but also exhibit superior characteristics compared to their bulk counterpart due to their reduced thickness (*1*), such as special adsorption behaviors (*2*) and enhanced thermal conductivity (*3-4*). Furthermore, BNNSs display distinct thickness-dependent properties from graphene and other 2D materials, such as unique mechanical response under indentation (*5*). Here, we present an overview of the thickness-related special properties of BNNSs, primarily derived from mechanically exfoliated *h*-BN single crystals. These properties span various domains, including Raman signatures (*6*), molecule adsorption-induced conformational changes (*2*), mechanical properties (*5*), thermal conductivity (*3-4*), and thermal expansion coefficients (*3*). Moreover, we also explore the underlying mechanisms governing these atomic-scale thickness effects. Leveraging their unique properties, we also investigates diverse applications of BNNSs, encompassing surface-enhanced Raman spectroscopy (*7*), metal-enhanced fluorescence (*8*), and isotropic thermal management (*9*).

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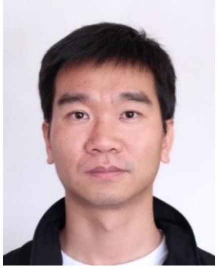
Presenter's Biography



Dr. Qiran Cai is currently a Research Fellow at the Institute for Frontier Materials, Deakin University, Australia. He obtained his Ph.D. in Materials Engineering from Deakin University in 2017. He has been awarded the Australian Research Council Discovery Early Career Researcher Award (DECRA). His research centers on investigating fundamental properties of two-dimensional materials, such as Raman signature, thermal conductivity, thermal expansion coefficient, and adsorption behaviour, as well as their application potential in surface-enhanced Raman spectroscopy, anti-oxidation coating, energy harvesting and thermal management.

Revolutionizing Activation Technology for Advanced Hierarchically Porous Carbon Materials

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Hierarchically porous carbon materials, with their micro-, meso-, and macropores, are critical to advancing a wide range of applications. However, traditional activation processes often produce inferior micropore-dominated structures or require extensive chemical use and complex, multi-step procedures to introduce mesoporisity that compromise material integrity and scalability. Emerging advanced fabrication methods, while promising, still face challenges in practicality and environmental impact. This research introduces a groundbreaking activation technology that revolutionizes the fabrication of hierarchically porous carbon using existing carbonization equipment. By leveraging controlled carbon-alkali metal complex formation and catalytic activation, we achieve precise and efficient transformation of diverse carbon precursors—from biomass to synthetic polymers—into novel nanostructured porous carbon materials. These include interconnected micro-meso-macro pores, graphene-like tubular forms, and wrinkled graphene-covered configurations. Our universal, scalable approach minimizes chemical use and maximizes process efficiency, setting a new benchmark in carbon material science. The resulting advanced porous carbon fibres, either as standalone materials or substrates, demonstrate exceptional performance in various applications, including energy storage, electrochemical CO_2 reduction, selective gas capture, and water purification, with a focus on bacteria and virus retention. This work addresses the limitations of current methods and paves the way for transformative innovations in carbon science, providing sustainable solutions with significant industrial and environmental benefits.

Biography

Dr. Quanxiang Li is an ARC DECRA Fellow at Deakin University, renowned for his pioneering work in carbon fibre and composite materials development. After earning his PhD from Deakin University in 2016, he was awarded the prestigious Alfred Deakin Postdoctoral Research Fellowship in 2019. His research is at the forefront of synthesizing porous carbon fibre materials with customized structures and functionalities, particularly for environmental and energy applications. Dr. Li is also an expert in sustainable manufacturing technologies for advanced carbon fibres and composites. As the lead inventor of a groundbreaking porous carbon-based technology and a commercialized composite filter cartridge, his innovations have made significant practival research and industry impacts. He has published over 60 peer-reviewed papers in top international journals, amassing more than 3,000 citations.

Graphene oxide membranes

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Our study presents graphene oxide (GO)-based membranes, precisely engineered for specific structure and morphology for enhanced water purification, selective gas separation, and moisture adsorption capabilities. Our investigation explores the water transport dynamics within cation-intercalated graphene oxide membranes, where the cations serve as moisture-attracting agents along the channel walls. Through systematic water transport experiments, we demonstrate that the slip length of the nanochannels exhibits an exponential decay relative to the hydrated diameter of the intercalated cations. In practical applications, we have effectively utilised our GO membrane to remove natural organic matter, humic substances, chlor(am-)ine and other contaminants from water, all while maintaining stable water flux rates. Throughout experiments, we monitored membrane stability, finding consistent performance over 4 weeks in our graphene oxide-based flat and hollow fibre membranes, ensuring sustained functionality. Our experimental results demonstrate the reliability of GO membranes, validating their suitability for long-term applications without compromising performance. Our experimental results demonstrate the reliability of GO membranes, validating their suitability for long-term applications without compromising performance. Our research paves the way for membrane-based innovative solutions for separation and purification with potential industrial applications.

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Presenter's Biography: Rakesh Joshi is an Associate Professor at the School of Materials Science and Engineering, leading the Graphene Research Group. He is the Theme Leader-Energy and Environment for the School of Materials Science and Engineering, UNSW. Before joining UNSW, he was a Marie Curie International Fellow with Nobel Laureate Sir Andre Geim at the University of Manchester. A/Prof Joshi is currently leading various industry-funded research projects on the application of graphene. Rakesh Joshi has over 115 journal articles (and 5 international patents), with over 85 articles as the first/lead author. Dr Joshi is among a select group of researchers worldwide whose work has been recognised through the award of the most prestigious relevant international research fellowships: the Marie Curie International Incoming Fellowship -2011 (European Union),(JSPS (Japan) Invitation Fellowship, an Alexander von Humboldt Fellowship, and a very recent VIABHAW Fellowship from the Government of India. He is a Fellow of the Royal Society of Chemistry.

Actuation, Mechanical Energy Harvesting, and Refrigeration Using Coiled or Plied Polymer or Carbon Nanotube Yarns

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The conversion of yarn twist to the twist of coiling, and the reverse, is important for our high-performance artificial muscles, mechanical energy harvesters, and twist-based refrigerators. We here describe the physical basis of each of these quite different devices, the differently needed structures for performance optimization, and some of their applications. Key issues are how we can modify the fabrication method and used material in order to optimize performance for specific application needs, as well as dual needs like a yarn that can perform as a muscle, mechanical energy harvester, and an energy storage device. In many cases, there are no presently known alternative methods for achieving the performance of our yarns. For example, for harvesting mechanical energy between 2 and 120 Hz, our most recent twistron carbon nanotube harvesters have higher gravimetric peak power and average power than previously reported for any prior-art, material-based mechanical energy harvester.

3D Printing of Liquid Metal Nanoparticle/Polymer Composites

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The integration of nanomaterials with 3D printing technologies has rapidly advanced, making significant strides in key biomedical fields such as regenerative medicine, tissue engineering, cancer research, and medical imaging. This combined approach offers a powerful strategy to address the limitations of both nanomaterials and 3D printing, driving innovations in material design and diverse applications.[1] In this talk, I will firstly introduce the surface engineering of liquid metal nanoparticle using RAFT polymers,[2-4] then focus the development of nanoparticle/polymer composites using state-of-the-art 3D printing techniques. I will also present our recent research on 3D-printed liquid metal polymer composites, highlighting their applications as near-infrared (NIR)-responsive 4D printed soft robots,[5] hybrid soft robots, and antibacterial scaffolds.

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Presenter's Biography

Bio: Ruirui Qiao is a Group Leader and NHMRC Emerging Leadership Fellow in Australian Institute for Bioengineering and Nanotechnology (AIBN), University of Queensland (UQ). She earned her PhD from the Chinese Academy of Sciences in 2014, along with an MSc in 2007 and a BSc in 2005 from Peking University, China. Leading a research group at AIBN, UQ, she is committed to advancing the field of functional polymer/inorganic nanohybrids for biomedical applications, including disease diagnosis, drug/gene delivery, tissue engineering, antibacterial solutions, and soft robotics. So far, she has published >110 refereed journal articles including Science, Nature Communications, ACS Nano, Advanced Materials, and JACS, with an H-index of 44 and >7000 citations. Among others, she currently serves as the associate editor for Science Advances (AAAS), Journal of Nanobiotechnology (Spring Nature) and Cancer Nanotechnology.

Green carbocatalysis for energy and chemical conversion

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Nowadays, energy crisis and environmental pollution are the important issues in the world. Novel catalysts based on green materials can provide innovation and benefits in materials and catalytic reactions. Currently, most of industrial catalysts are metal-based materials, which are both expensive and toxic to the environment. Carbon is the richest element on the earth and can be employed as an alternative to metals as catalysts. Catalytic reactions using carbon materials have been an important technique for energy conversion, chemical synthesis and environmental remediation. Compared with metal-based catalysts, carbonaceous materials are identified as more sustainable catalysts due to the "green" nature in avoiding potential secondary contamination by metal leaching.

In the past years, we have prepared different carbon-based materials and investigated their catalytic performances in various reactions, such as electrochemical oxygen reduction, advanced oxidation, and selective oxidation. We have modified the structure and chemical functionality of carbons to understand the role of defects and functional groups as well as their integration in catalysis. In general, those materials have demonstrated effective performance and their structural defect and functional groups will affect the performance.

Presenter's Biography

Prof. Shaobin Wang obtained the degrees of BSc and MSc in Chemistry from Peking University and PhD in Chemical Engineering from the University of Queensland (Australia). He has been a John Curtin Distinguished Professor at Curtin University (Australia) and is now a Laureate Professor at the School of Chemical Engineering, the University of Adelaide (Australia). His research interests focus on nanomaterial synthesis and application for adsorption and catalysis, fuel and energy conversion and environmental remediation. He was awarded 2012 Thomson Reuters Citation & Innovation Awards in Australia and is listed as a highly cited researcher in Engineering, Chemistry and Environment & Ecology in 2016-2022. He is a co-editor of Journal of Colloid and Interface Science and an editor of Applied Catalysis B: Environmental as well as an editorial board member of several international journals.

Mapping Atomic Scale Electronic Structures of Carbon Materials for Energy and Quantum Sensing Applications

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Electron Energy Loss Spectroscopy (EELS) in Scanning Transmission Electron Microscopy (STEM) is a powerful tool for mapping atomic-scale electronic structures, thanks to the sub-0.1nm spatial resolution enabled by STEM. My group has been developing methods using EELS to detect and locate defects in carbon-based materials with a focus on the quantum sensing and energy technologies.

For quantum sensing, our work is focused on fluorescent nanodiamonds (FNDs), diamond nanoparticles containing so-called color-centers which are composed one substitutional dopant atom paired with a lattice vacancy. They draw widespread attention due to their exceptional optical and spin properties, making them excellent candidates for room-temperature quantum sensing. However the advancement of FND requires atomic scale understanding of the crystallographic environment around the defect centres as well as the surface properties. These factors are critical for their fluorescent brightness and optical stability. Using a combination of density functional based EELS calculations and electron scattering calculations, we have pinpoint the locations of these atomic defects [1,2] at sub-nm resolution[3].

For energy applications, single atom catalysts (SACs) within a carbon material based support are known to mediate electrochemical CO_2 reduction reaction (CO2RR). However, how the metal atom/clusters and the carbon-based support interact to catalyze CO2RR is not well understood. Here STEM-EELS allows us to probe the local interaction of doped graphene[4] and carbon nitride with single transition metal atom/clusters. Such information is important in answering the key issues of activity and product selectivity.

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Biography

Shery Chang is an Associate Director of Electron Microscope Unit, Mark Wainwright Analytical Centre and Associate Professor at School of Materials Science and Engineering, UNSW. Her expertise is advanced transmission electron microsocpe and spectroscopy to study surface, defect and interfaces of nanomaterials and thin films, in particular new diamond mateirals for quantum sensing and perovskite for energy applications.

Rationally Designed 3D Carbon Networks for Li-O_2 Batteries with Ultra-High Energy and Power Densities

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Abstract

As the demand for sophisticated energy storage solutions grows, the lithium-oxygen (Li-O_2) battery emerges as a leading candidate, noted for its impressive theoretical energy density. However, its practical use at high power densities is impeded by pronounced declines in capacity, primarily stemming from the tortuous pathways within the porous cathode materials that restrict the mass transport kinetics. Additionally, the lack of readily accessible space for storing discharge products serves as another critical rate-limiting factor. Designing conductive cathode architectures containing ordered and straight tunnels is supposed to be an effective strategy to relieve this issue. Herein, we rationally design a 3D interconnected covalent-bonded graphene-CNT (G-CNT) network via an AAO/Al foam. The architecture of the 3D network consists of vertically aligned CNTs with open-end tips that are seamlessly connected with a holey graphene layer. The unique structure can facilitate rapid ion/O_2 transport and the well-defined interconnected space among G-CNT can effectively host the discharge products at high current density. Moreover, the easy functionalization could endow the prepared G-CNT network with high catalytic ability. The resulting S, N co-doped G-CNT networks demonstrate decent concurrent energy and power density ranging from 1 A g^{-1} to 40 A g^{-1} with yielding considerably high capacities from 61,841 mAh g^{-1} to 12,663 mAh g^{-1} accordingly. This corresponds to a highest specific energy of 170.6 kWh $kg^{-1}_{\text{active materials}}$ and power density of 96.8 kW $kg^{-1}_{\text{active materials}}$, respectively. The transformation of Li_2O_2 from a film-like to a sheet-like configuration during discharge appears to play a pivotal role in enabling the remarkably high-power density observed. The novel G-CNT networks broaden the versatility of carbon materials for energy storage and may expand the killer applications of Li-O_2 battery to electric vehicles and power tools due to the excellent power output.

Presenter's Biography

Dr. Shuangyue Wang earned his Ph.D. degree from the University of New South Wales (UNSW) in 2022, under the guidance of Prof. Sean Li. He is currently serving as a Postdoctoral Research Fellow in the School of Chemical Engineering at UNSW, supervised by Prof. Liming Dai. During his Ph.D. studies, he focused primarily on the growth of advanced 2D materials and the deposition of ultrathin metal films. Currently, his research is directed towards the fabrication of multifunctional and multidimensional carbon materials and their applications in energy conversion and storage. Dr. Wang has demonstrated significant capabilities and gained extensive experience in the growth of carbon materials and the design of 3D carbon structures. His ongoing projects aim to develop innovative cathode carbon materials for advanced energy storage systems and novel metal-free electrocatalysts for energy conversion.

Multiphysical Coupled Microdesign for Sustainable Zinc-Based Batteries

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To tackle the critical challenge of poor structural stability in electrode materials caused by carrier intercalation and deintercalation in aqueous zinc-ion batteries, we employed defect engineering to regulate the size and shape of micro-nano crystal tunnels. Additionally, doping was utilized to control the migration rate and type of carriers, achieving ultra-long cycle applications under high rates for aqueous batteries. Concerning the core challenges of low energy density and low power density due to sluggish kinetics in zinc-air batteries, we developed a multi-field responsive ORR/OER bifunctional high-entropy alloy nanocatalyst with high activity and stability. We also designed and constructed a novel battery structure with multi-field synergistic enhancement, significantly improving the specific energy and rate capability of zinc-air batteries.

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Presenter's Biography

Dr. Shun Wang, male, second-level professor of the state, Ph.D supervisor, he is now the vice president of Wenzhou University, State-Council Allowance Obtained Expert, National Young and Middle-aged Experts with Outstanding Contribution, and the editor-in-chief of a Wiley's journal Carbon Energy with an impact factor (IF) of 21.556. He is a Fellow of the Royal Society of Chemistry (FRSC), head of National Talent Introduction Demonstration Base, director of chemistry doctoral program, director of Zhejiang International Science and Technology Cooperation Base for Micro/Nano Structured Carbon Materials Technology, director of Zhejiang Engineering Research Center of Electrochemical Energy Materials and Device, dean of the Institute of New Materials and Industrial Technologies, and member of Zhijiang Talents Association for Science and Technology.

His research efforts have been dedicated to the novel design, preparation, and multi-dimensional assembly of carbon energy materials, fluoro-materials and engineering, from the fundamental research aspects of structure-activity relationship to the applicable exploration of their efficient energy storage and functional polymers. He has published more than 180 papers on high level of international journals, such as Nat. Commun., ***Nat. Sustain., Chem. Soc. Rev., Adv. Mater., Energy Environ. Sci., J. Am. Chem. Soc., Angew. Chem. Int. Ed.,*** etc. with a H index of 44. He filed 2 international PCT patents with 1 US authorized. He also filed 180 Chinese patents with 90 authorized. More than 10 patens have been licensed to industry for products development. He has organized and served as the president and vice president of international academic conferences for many times, and was invited to give more than 100 reports at international and domestic conferences, universities and scientific research institutes.

Synthesis of polymer/GO nanocomposite foams via miniemulsion polymerization and freeze-casting techniques

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Lightweight and porous carbon-based polymeric foams have attracted significant attention for their attractive properties, which enables application in multidiverse domains. Polymer nanocomposite foams with graphene oxide (GO) in particular is an intriguing class of material that combines the synergistic interactions between polymer with GO, resulting in the emergence of new sophisticated materials. An increase in research efforts have been observed in designing waterborne, yet strong and highly recoverable polymeric foams in response to persisting environmental issues. In the present work, we demonstrate a novel method which is an efficient one-pot green approach to prepare polymer/GO foam from a dispersed phase – this is in great contrast to the high internal phase emulsion (polyHIPE) method, which employs the continuous phase as the porous monolith.[1] Polymer nanocomposite reinforced with GO were synthesised via miniemulsion polymerization (oil-in-water system), followed by freeze casting to obtain a hybrid nanocomposite foam. The as prepared polymer/GO foams exhibited a dense porous lamellar microstructure that possesses recoverable elasticity and excellent mechanical behaviour. The stability in water, oleophilicity and pore-rich properties of this sponge-like architecture as an oil absorbant material, particularly for oil-spills cleaning, will also be discussed.

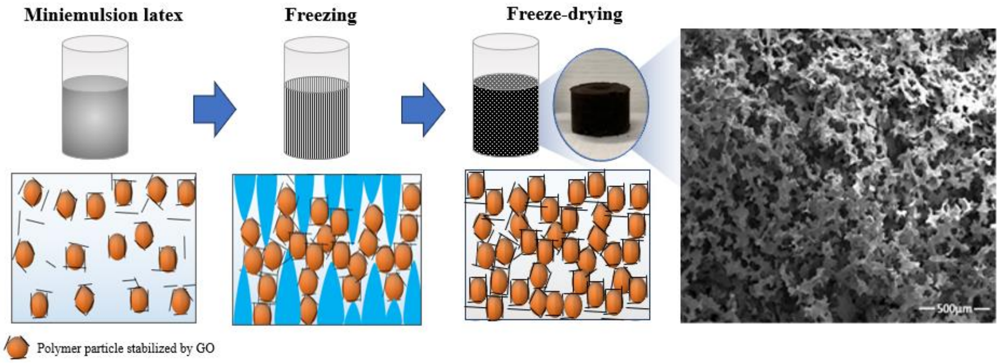

Figure 1. Schematic diagram of polymer/GO nanocomposite foam fabrication via miniemulsion and freeze casting.

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Multilayered Graphene Membrane for Ammonium-ion Storage

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Abstract

Ammonium-ion (NH_4^+) energy storage systems present a promising avenue for large-scale, inherently safer energy storage. Unlike metallic ions, which typically exhibit spherical geometries, NH_4^+ ions possess a tetrahedral structure[1]. This unique geometry facilitates selective intercalation within electrode materials, potentially enhancing power density and improving cycling stability[2]. However, one of the primary challenges in this technology lies in developing electrode materials capable of effectively and reversibly accommodating NH_4^+ ions, which is crucial for achieving high-performance energy storage. In this study, we investigated the tuning of porosity in multilayered graphene membranes (MGM) to optimize the interlayer spacing for NH_4^+ ion intercalation. Characterization of the MGM revealed a stacked architecture with a large surface area. The amorphous nature of the graphene membrane provided oxygen vacancy sites, enabling flexible hydrogen bond formation between the graphene layers and NH_4^+ ions. Electrochemical characterization of the MGM, using a 1 M $(NH_4)_2SO_4$ electrolyte, demonstrated electric double-layer capacitance. The membrane operated within a voltage window of up to 1 V, delivering a maximum capacitance of 258 F g^{-1} at a current density of 2 A g^{-1}. Additionally, the membrane exhibited exceptional long-term stability, with 100% capacitance retention after 72 hours of floating and 1000 continuous charge-discharge cycles, effectively addressing the cycling stability challenges of NH_4^+ ion storage.

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Presenter's Biography

Syam completed his PhD at Universiti Malaysia Pahang in 2017. Following his doctorate, he worked as a Chemist at GeoChem Middle East, Fujairah, before resuming his research career in 2019 as a Research Fellow at Sunway University, Malaysia. In 2021, he migrated to Australia and served as a Postdoctoral Research Fellow at Queensland University of Technology (QUT), Brisbane. Currently, he is a Research Fellow in the Department of Chemical Engineering at the University of Melbourne, working on an ITTC research project. His research interests focus on the development of sustainable materials for energy storage devices, the recovery of materials from spent batteries, and redox flow batteries. Syam has successfully completed two industrial projects, published over 40 research papers, edited a book, and is an active reviewer for several international journals..

Electrooxidative decarboxlyation of volitile fatty acids to hydrocarbons using high entropy metal phosphides

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Abstract

The conversion of volatile fatty acids (VFAs) to larger alkanes through electrooxidative decarboxylation (also known as Kolbe coupling) provides a sustainable route toward high density fuel production. This is especial true when considering the difficulties of converting VFAs from biomass into fuels given complications in separation technologies and traditional thermal catalytic conversions methods. Though promising, electrochemical pathways for VFA coupling traditionally employ a range of undesirable characteristics, including high cell voltage (> 4V), overuse of Pt group metals (PGM), and/or incorporation of organic solvents over water.

In this study we investigate the electrochemical performance of non-PGM based high entropy metal phosphide (HEMPs) catalyst for the conversion of hexanoic acid under neutral pH conditions. Our results show that high entropy materials performs better compared to mono, bimetallic, and trimetallic counterparts and requires lower over potential voltage (2.31V) to produce coupled products as well as phase separation occur during the reaction. Furthermore, various in-situ synchrotron methods were used to demonstrate structure property relationships that help to establish the rational for the excellent properties observed in high entropy catalysts..

Tanveer Ahmad is currently a PhD candidate at the School of Chemical Engineering, University of New South Wales, Australia. His current research interests focus on carbon based advance nanomaterials for electrochemical energy technologies.

Exploring photofunctional materials at the nanoscale

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Photofunctional materials, which convert light energy into other forms of energy, play a crucial role in solar energy harvesting, hydrogen generation, and optomechanical devices. These materials rely on the generation and separation of photo-excited charge carriers, as well as their interactions with other physical properties such as electrical polarization and phonons. To enhance the understanding, design, and development of photofunctional materials, it is crucial to investigate photo-induced effects at different length scales, particularly at the nanoscale. We have successfully developed photo-atomic force microscopy (pAFM), which can *in situ* characterize nanoscale photo-induced behaviors and correlate them with the materials' morphology and structures. The customized pAFM has helped uncover intriguing phenomena and understand mechanisms in various material systems. For example, it has shown the interaction between photo-induced charges and polarization in ferroelectric materials,[1] discovered how local strain enhances photoconductivity in 2D materials,[2] and revealed the effects of phase separation on photovoltaic properties in hybrid perovskites.[3] The nanoscale photoinduced effects characterised by the pAFM provide new insights into the photofunctionality, which will help enhance performance in applications such as photocatalysts, photovoltaics, sensors, and optoelectronic devices.

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Presenter's Biography

Dr. Teng Lu earned his PhD from the Australian National University (ANU) in 2018 and continued there as a Research Fellow. He is currently an ARC Discovery Early Career Researcher Award (DECRA) fellow at ANU. His research began with polar functional materials, exploring how their structure-property relationships evolve under external stimuli, with applications in energy storage, conversion, and harvesting. He is particularly interested in complex structural analyses across various length scales (from average to local) and time scales (from static to dynamic) using electron, neutron, and synchrotron X-ray scattering techniques. His work also involves characterizing nanoscale functionalities through scanning probe microscopy (SPM) techniques and developing new methods to map local properties under different external conditions.

Micro- and Nanoengineering of Semiconductor Materials for Biosensing

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Semiconductors hold great promise for a range of sensing devices [1], but their applications for sensing biological systems are limited by their inherent sensing performance [2]. In this talk, I will present our work on the micro- and nanofabrication of semiconductor materials to create micro/nanostructures with enhanced physical sensing effects [3,4]. I will also discuss our recent interventions using a phonon-enhanced coupling mechanism to enhance the sensitivity of semiconductor sensors by several orders of magnitude compared to conventional sensors [5,6]. I will showcase the capability of the fabricated nanostructures in interacting with biological systems, potentially for wearable applications on the skin and for use inside the body [7,8].

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Presenter's Biography: Toan Dinh is currently an Associate Professor in the School of Engineering and affiliated with Centre for Future Materials and Centre for Health Research at the University of Southern Queensland (UniSQ), Australia. He received his Ph.D. from the Griffith University in 2017, followed by a postdoctoral training program before joining UniSQ in 2019 as a Lecturer (Assistant Professor). His research aims to enhance the understanding of semiconductor properties at different length scales and transform these rigid materials into flexible and wearable sensors that can interact with biological systems, enabling more accurate monitoring of human health

Liquid metal chemistry towards CO_2 reduction and other catalytic reactions

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Liquid metals are an emerging class of compounds that are liquid close to room temperature yet exhibit metallic conductivity [1]. Liquid metals have found application in the design of flexible and reconfigurable electronics and more recently emerged as a platform for the synthesis of nano-structures [2] as well as a unique class of catalysts that is extraordinarily resilient towards deactivation [3]. In comparison to other liquids such as covalent solvents and ionic liquids, comparatively little is known about the chemistry that occurs inside molten metals. This talk covers the emerging picture of liquid metal chemistry and will report our most recent results on the fundamental processes that govern the behaviour of liquid metals. Following this, our work in the area of CO_2 electroreduction, chemical looping of liquid metals to turn CO_2 into graphene [4] and the synthesis of NH_3 [5] will be covered.

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Presenter's Biography

Dr. Torben Daeneke is a Professor within the School of Engineering at RMIT University. His early research focussed on charge transfer processes in dye sensitised solar cells. After joining RMIT he shifted his attention towards the synthesis and application of two-dimensional materials for electronics applications. Durign this time he commenced work on liquid metal solvents and their use in nanomaterials synthesis. Now, his research is focused on liquid metal chemistry more broadly, where he is exploring fundamental phenomena as well as applications in synthesis, electronics and catalysis. Prof. Daeneke currently leads a research group of 17 HDR students and 5 postdoctoral fellows. He is a former ARC DECRA fellow (DE2019) and has published over 140 peer reviewed journal articles.

Neutron imaging applications in carbon fiber, battery and cement research

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The neutron radiography / tomography / imaging instrument DINGO is operational since October 2014 to support research at ANSTO. DINGO had a high subscription rate from a broad national and international scientific user community and for routine quality control for defense, industrial, cultural heritage and archaeology applications. A large part of the user community is utilizing neutron imaging to analyze carbon fiber products, running in situ-battery imaging, monitor water intake of new cement paste. All three types of experiment have the goal to reduce the CO2 footprint of modern societies. Neutron imaging differs from the standard x-ray methods mainly, because of its high penetration depth and the sensitivity to light elements, light Hydrogen and Lithium. The strong penetration depth makes it ideal to run in-situ experiments under non ambient conditions like high pressure or temperature. At ACNS (Australian Center for Neutron Scattering) we provide an impressive suite of sample environment to meet the needs of our scientific community. It includes cryostats, furnaces battery control and high pressure setups. The neutron imaging instrument DINGO provides a large variety of instrument settings to address the size and resolution requirements. DINGO offers pixel sizes from 1.75µm - 80µm and a maximum field of view of 200 x 200 mm2, with a main setting of around 15-30µm pixel size. Modern large astronomy cameras provide 26MP to enable larger sample size combined with high resolution settings. Fast imaging of up to a full tomography in 2-5 minutes with reduced resolution is feasible as well. I will provide an overview of successful neutron imaging experiments in the field of carbon science to showcase the potential of that methods.

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Presenter’s Biography

A/Prof Dr. Ulf Garbe got his PhD in 2005 at Georg-August-University of Goettingen, Centre for Geoscience, Germany, started his career as a graduate Mineralogist (Dipl.-Min) and focused on material science at large research facilities. Currently, he is employed as an instrument scientist for neutron imaging at ANCS. He established the neutron imaging community as a pioneer through engagement with Australian universities on a national level and through board membership and later as president of the ISNR (International Society for Neutron Radiography).

Advancing Clean Energy: Metal free Carbon-Based Catalyst for Sustainable electrocatalytic Urea synthesis

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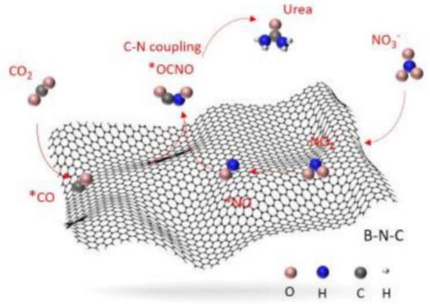
Metal-based catalysts, despite their high catalytic performance, face critical limitations such as limited availability, high cost, low selectivity, and insufficient durability, making them less viable for large-scale, commercial applications. To address these challenges, this study explores carbon-based catalysts, which offer significant advantages, including abundance, affordability, and tunable chemical properties that can be optimized for diverse energy-related applications.



Specifically, we focused on the promising application of carbon-based catalysts in the electrocatalytic synthesis of urea through the co-reduction of CO_2 and NO_3, a process with potential to replace energy-intensive traditional methods. We emphasize the need to advance the understanding of reaction mechanisms, catalytic active sites, and strategies to boost catalytic performance in carbon-based systems. put forward. Thus, this work provides new sights into the catalyst design and the reaction mechanisms, and the co improvement of NO_3RR and CO_2RR activities is expected to be the further development direction towards electrocatalytic urea synthesis.

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VANDANA VERMA, PhD candidate, Center of Advanced Carbon Materials, School of Chemical Engineering, University of New South Wales, Sydney . My research intersts include Metal free carbon based catalysts for various electrochemical applications.

Directional Synthesis of Rare Earth Materials and Analysis of Spatiotemporal Dynamic Mechanisms

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Abstract：The advancement of industrial alkaline water electrolysis (AWE) technology is primarily hindered by the limited adsorption coverage of anodic OH^- under high current density conditions, leading to changes in surface microenvironment pH value and a decrease in oxygen-containing active species. To address these scientific challenges, we have developed a controlled synthesis method utilizing rare earth ions for the directional construction of rare earth-modified NiS_2 catalysts. The interface formation process between rare earth particles has been elucidated through in-situ infrared and in-situ fluorescence spectra during the synthesis process. By employing multiple in situ spectroscopy techniques including isotope-labeled experiments and time-resolved absorption spectroscopy, we have established the relationship among OH^- coverage, active site density, and catalytic activity based on a series of rare earth-modified NiS_2 materials. Furthermore, the stability of operating conditions has been verified for over 100 hours using a kW-level AWE device. This research provides novel insights into rare earth modification as a potential solution to enhance anodic OH^- coverage.

Keywords：Rare earth, Distributed state control, Catalytic reaction, In situ dynamic characterization, Industrial alkaline electrolyzed water

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Sulfur Containing Organic Molecular Additives for Zinc Metal Anode Modification

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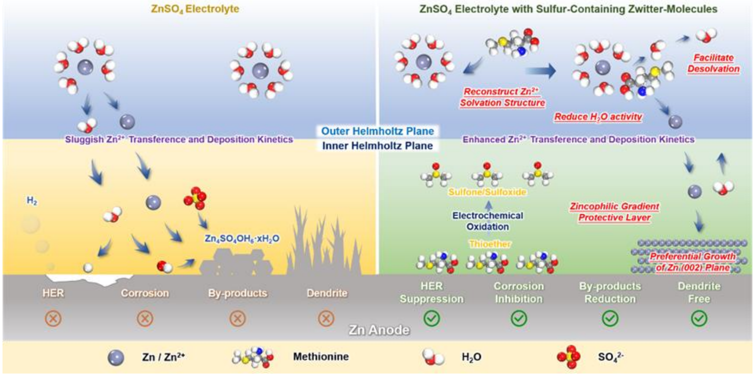
Abstract

Numerous organic electrolyte additives have been reported to improve Zn anode performance in aqueous Zn metal batteries (AZMBs). However, the modification mechanism needs to be further revealed in consideration of different environment for electrolyte and electrode during charge-discharge process. Herein, sulfur-containing zwitter-molecule (methionine, Met) is used as an efficient additive for $ZnSO_4$ electrolyte. In electrolyte, Met reduces the H_2O coordination number and facilitates desolvation process by virtue of its functional groups (-COOH, $-NH_2$, C-S-C), accelerating Zn^{2+} transference kinetics and decreasing the amount of active water. On electrode, Met prefers to adsorb on Zn (002) plane and further transforms into a zincophilic protective layer containing C-SO_x-C through an in situ electrochemical oxidization, suppressing H_2 evolution/corrosion reactions and guiding dendrite-free Zn deposition. By using Met-containing $ZnSO_4$ electrolyte, the Zn//Zn cells show superior cycling performance under high currents and capacities (up to 30 mA cm^{-2}/30 mA h cm^{-2}) with large depth of discharge (54%). Moreover, the Zn//$NH_4V_4O_{10}$ full cells using the modified electrolyte exhibit good performance at temperatures from -8 to 60 ° C. Notably, a high energy density of 105.30 W h kg^{-1} can be delivered using a low N/P ratio of 1.2, showing a promising prospect of Met electrolyte additives for practical use.



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Presenter's Biography

2016-2020	Beijing University of Chemical Technology	Bachelor of Engineering
2020-	Beijing University of Chemical Technology	Doctoral Student

Advancing carbon-neutral and negative construction materials through nanotechnology and carbon sequestration

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This paper reviews the mechanisms of carbon sequestration, testing methods for carbon sequestration capacity, and the performance of novel construction materials, including wollastonite, titanium dioxide nanoparticles (Nano-TiO_2), graphene oxide (GO), biochar, and cellulose fibers (CS), as well as their performance in cement-based materials. The development of a system boundary model allows for a comprehensive analysis of the environmental impact of the preparation of these materials as new functional concretes. It is demonstrated that wollastonite can react with atmospheric carbon dioxide (CO_2) to form carbonate minerals for carbon sequestration. Nano-TiO_2 and GO adsorb and transform CO_2 by using light-excited charge carriers to generate redox reactions and oxide functional groups on their surfaces and edges, respectively. Biochar relies on its physical and chemical stability for carbon sequestration, whereas the mechanism of carbon sequestration in cellulose fibers is related to their plant structural properties. In cement-based materials, wollastonite significantly enhances mechanical properties by filling pores and bridging microcracks. Nano-TiO_2 and GO enhance the mechanical properties by providing nucleation sites and template effects, among other mechanisms. An appropriate amount of biochar improves densification and strength, while plant fibers facilitate the hydration process of cement, thus improving mechanical properties. Furthermore, Life Cycle Assessment (LCA) analyses have demonstrated that wollastonite and cellulose fibers possess considerable environmental benefits in the production of low-carbon concrete due to their low Global Warming Potential (GWP) and low potential for negative impacts on the environment and humanity. By examining the current state of development of carbon-neutral and carbon-negative construction materials, this review emphasizes the pivotal role of these novel sustainable construction materials in combating climate change.

Keywords: Carbon sequestration; Nano-TiO_2; Graphene oxide; Wollastonite; Biochar, Cellulose fiber

Wengui Li is a Scientia Associate Professor in the School of Civil and Environmental Engineering and the group leader of Intelligent Concrete and Infrastructure Materials in the Centre for Infrastructure Engineering and Safety (CIES) at The University of New South Wales (UNSW Sydney), Australia. He is the recipient of Australian Research Council (ARC) Future Fellow and ARC DECRA Fellow.

Anomalous ion transport in electrified graphene membranes

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The ability to modulate electronic charge transport at electroactive material interfaces through external voltages is fundamental to the revolutionary advancements in transistor technology, crucial for modern information processing and intelligence systems. Drawing inspiration from the immense success of microelectronics and the critical role of electrical signalling by ionic charges in biological systems, there is burgeoning interest in harnessing external voltages to control ion transport at electronic/ionic interfaces or under nanoconfinement, aiming to create novel iontronic devices not just for neuromorphic computing, but also for energy harvesting and storage, energy-efficient ion separation and beyond. However, investigating ion transport along electrified electronic conductor interfaces remains experimentally challenging. Here, we report an interface amplification strategy to examine the influence of external voltage on lateral cation-anion correlated ion transport, specifically ambipolar ion diffusion across electrified interfaces consisting of electronically conductive and multilayer-cascaded reduced graphene oxide (rGO) membranes. We found that while the remaining negatively charged chemical groups on rGO typically impede ion permeation compared to bulk solutions, applying a negative external voltage enables unexpectedly rapid and collective permeation of both cations and anions through the membranes, with effective diffusion coefficients up to three orders of magnitude higher than bulk. Our findings not only shed light on the unsolved questions about ionic structure and resulted transport at electrochemical interfaces with high charge density, but also provide new insights into the development of advanced electrochemical and iontronic technologies.

Presenter's Biography

Dr. Wen-Jie Jiang is an ARC DECRA Fellow in Materials Science and Engineering at the Department of Chemical Engineering, University of Melbourne (UoM), Australia. He earned his PhD in Physical Chemistry from the Institute of Chemistry, Chinese Academy of Sciences (ICCAS) in 2017, under the mentorship of Prof. Li-Jun Wan and Prof. Jin-Song Hu. Dr. Jiang's research centres on the design of electrocatalyst materials and the regulation of ion atmospheres at electrochemical interfaces. His work aims to advance efficient and precise small molecule electrosynthesis and address ion transport challenges, including ion sieving, seawater deionisation, and metal element recovery. He has published 70 papers in leading journals across energy, materials, catalysis, and chemistry, including *Acc. Chem. Res.*, *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*, *Adv. Mater.*, *Adv. Energy Mater.*, *Adv. Funct. Mater.*, and *ACS Catal.* His publications have garnered over 9,000 citations, reflecting an H-index of 46. Dr. Jiang's contributions have been recognized with several prestigious awards, such as the World's Top 2% Scientists (Stanford University), National Postdoctoral Program for Innovative Talents (China), Chinese Academy of Sciences President's Award for Excellence, and Outstanding Postdoctoral Fellowship (University of Melbourne).

Intelligent Wearable Resistive Skins for Monitoring Human and Organoids

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In the context of telehealth and internet of things (IOT), there are unprecedented needs for developing remote diagnostic tools that can monitor chemical and biological markers remotely anytime anywhere, such as via a smart phone. Such sensing devices are ideally soft and thin so that they can "bio-friendly" interface with soft biological systems. In this talk, I will present our skin-like sensing devices that can remotely monitor human's health and cardiac organoids.

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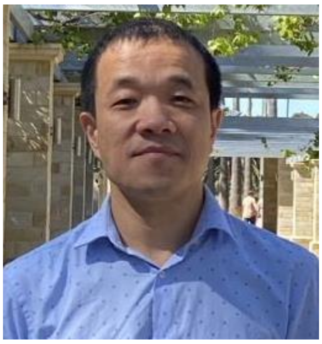

Wenlong Cheng is a professor in the School of Biomedical Engineering at the University of Sydney. He was a director of research in the Department of Chemical&Biological Engineering at Monash University, Australia. He is currently NHMRC Investigator Leadership Fellow and a fellow of Royal Society of Chemistry and was an Ambassador Tech Fellow in Melbourne Centre for Nanofabrication. He earned his PhD from Chinese Academy of Sciences in 2005 and his BS from Jilin University, China in 1999. He was Alexander von Humboldt fellow in the Max Planck Institute of Microstructure Physics and a research associate in the Department of Biological and Environmental Engineering of Cornell University. He founded Monash NanoBionics lab at the Monash University in 2010. His research interest lies at the Nano-Bio Interface, particularly self-assembly of 2D plasmonic nanomaterials, DNA nanotechnology, electronic skins and stretchable energy devices. He has published >200 papers. He is currently the scientific editor for Nanoscale Horizon (Royal Society of Chemistry) and the editorial board members for a few journals including Nanoscale, Nanoscale Horizons, Nanoscale Advances, Advanced Sensor Research, Advanced Electronic Materials, ChemNanomat, Advanced Sensors and Energy Materials, *i*Science, Chemosensors, and Austin Journal of Biomedical Engineering, FlexTech and Wearable Electronics.

Controllable Modification of Tip-Rich Carbon Nanotubes for Highly Selective Electrosynthesis of Hydrogen Peroxide

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Abstract

Hydrogen peroxide (H_2O_2) is an essential chemical widely applied in environmental treatment, chemical processing, and healthcare, with increasing demand driven by its role in public health and industrial processes.[1,2] However, the traditional anthraquinone process for H_2O_2 production is not only energy-intensive but also generates significant waste and faces safety concerns due to H_2O_2's instability during transport and storage.[3] In this study, we propose an alternative, sustainable approach for H_2O_2 electrosynthesis through the two-electron oxygen reduction reaction (ORR) by designing nitrogen-doped carbon nanotubes (CNTs) with a focus on tip-selective modification. Using a silica-coating and ball-milling strategy, nitrogen doping was concentrated at the CNT tips, optimizing the two-electron ORR pathway and achieving over 90% selectivity towards H_2O_2. The tip-enriched nitrogen configuration demonstrated superior catalytic performance and long-term stability, addressing limitations found in conventional metal-free catalysts. This work highlights the critical role of controlled nitrogen placement in enhancing catalyst activity and selectivity, paving the way for efficient, on-site H_2O_2 production. Our findings provide a basis for developing advanced carbon-based electrocatalysts aimed at sustainable energy and environmental applications, demonstrating a viable pathway for high-performance, metal-free catalysis.

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3. B. Q. Li, C. X. Zhao, J. N. Liu, Q. Zhang, *Advanced Materials* **2019**, 31, 1808173.

Presenter's Biography

Xiang Ao is a postdoctoral researcher at the School of Chemical Engineering, University of New South Wales (UNSW), Australia. He received his bachelor's degree in Optoelectronic Materials and Devices in 2015 and completed his PhD in Physical Electronics in 2021, both at Huazhong University of Science and Technology, China. During his PhD, he was also a visiting researcher at Georgia Institute of Technology, USA. Before his current position at UNSW, he conducted postdoctoral research at Yonsei University in South Korea. His research focuses on designing and synthesizing advanced electrocatalysts for energy storage and conversion, with applications in lithium-ion batteries, fuel cells, and sustainable chemical synthesis.

Engineered Carbon Catalysts for Green Hydrogen Peroxide Production and Environmental Application

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Photocatalysis hydrogen peroxide (H_2O_2) production has gained broad research attention since it is a potentially viable route for "green" on-site H_2O_2 manufacturing from just water and oxygen using renewable solar energy [1],[2]. In the past decade, stunning progress has been made. However, efficient photocatalysts are still in need to push the current boundaries of H_2O_2 production in terms of generation rate and product concentration [3]. Besides, a fit-for-purpose application is in need to demonstrate its practical use. In this presentation, we will talk our recent works on the rational design of photocatalysts for improved H_2O_2 production [4-6]. Additionally, the application for disinfection of bacteria in water will also be covered. It is expected to provide insights on designing photocatalysts with judicious structures and function for environmental applications via green photocatalysis process.

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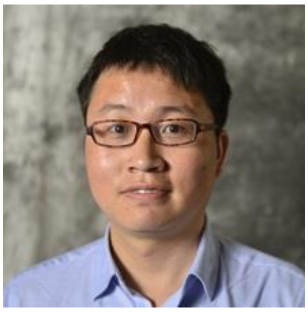
Biography



Dr. Xiangkang Zeng is an ARC DECRA Research Fellow at UQ Dow Centre for for Sustainable Engineering Innovation, School of Chemical Engineering, The University of Queensland. He obtained his PhD degree (Chemical Engineering) from Monash University Australia in 2017. He worked at the Hong Kong University of Science and Technology (HKUST) for postdoc research training from 2017 to 2018. He was a Postdoctoral Research Fellow in the Department of Chemical Engineering Monash University Australia from November 2018 to July 2022. His current research interest mainly focuses on the development of two-dimensional functional materials as advacned catalysts for hydrogen peroxide production, water treatment and antibacterial purpose. He has published more than 40 papers in prestigious journals, including Nature Communications, Advanced Energy Materials, Advanced Functional Materials, Angewandte Chemie, ACS Catalysis, Applied Catalysis B:Environmental, and Green Chemistry etc.

Carbon Nanohybrids for Catalytic Water Purification

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In this work, we will develop a series of carbon-based nanocomposites to address the inherent limitations of conventional carbonaceous materials in stability and efficiency. The structure and surface engineered carbon@carbon and carbon@metal composites will be engaged in the activation of peroxymonosulfate for generation reactive radicals and nonradical species to remove the micropollutants in water. Deliberate materials design, advanced characterisations and theoretical computations will be conducted to enable mechanism insights into the synergy of interfacial coupling and electron communication of composite materials toward enhanced catalysis, activity and stability. This study will provide a family of robust and highly reactive carbon composites for environmental remediation and other catalytic applications.

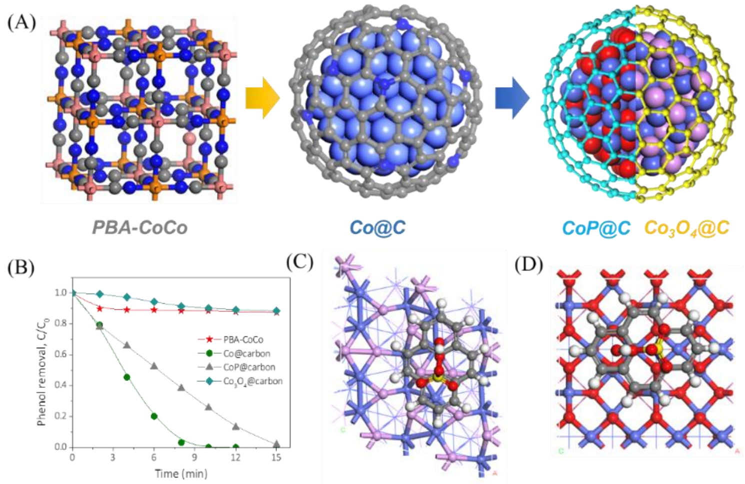

Figure 1.1 Synthesis and applications of carbon nanocomposites for water purification.

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Presenter's Biography

Dr. Xiaoguang Duan is an Associate Professor and ARC Future Fellow at School of Chemical Engineering of UoAdelaide. His research areas focus on environmental science and technology, green catalysis, and nanomaterials. He has secured over 2.4 M research income from Australian Research Council (DECRA, FT-level2, two DPs, and one LIEF), NCI, ANSTO, and UoA. Dr Duan have produced over 200 publications, including over 70 ESI Highly Cited Papers (Top 1%). Duan has received an h-index of 90 and a total of 30,000 citations (Web of Science). He was recognized as a Global Highly Cited Researcher in Environment/Ecology and Chemistry in 2022-2023 and in Cross-Field in 2020-2021. He was selected by The Australian annual research report as Top 40 Rising Stars in 2018-2021. He has been awarded the ACS Catalysis Early

Career Award, JMCA Emerging Investigator, ES&T Best Paper Award in Technology. Lately, Dr Duan was selected as the MIT Technology Review Innovators Under 35 Award and received prestigious ES&T James J. Morgan Award from American Chemical Society.

Mechanistic Insights into Small Molecule Electrocatalytic Conversion and Rational Catalyst Design

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Electrocatalysis enables the conversion, storage, and utilization of electrical and chemical energy, playing a crucial role in advancing renewable energy technologies. High-performance catalysts are essential for improving the efficiency of electrocatalytic energy conversion and reducing energy consumption. The electrocatalytic reaction process and its local catalytic environment are highly complex. The activity of catalysts is influenced not only by the surface and interfacial properties of the material but also by electrochemical interface factors such as electrode potential, solvent effects, and pH, which significantly impact the thermodynamics and kinetics of the reactions. By utilizing advanced simulation techniques, we have conducted extensive research aimed at designing high-active, low-cost catalysts and elucidating the reaction mechanisms involved in the electrocatalytic conversion of small molecules such as O_2, CO_2, and N_2.[1-4]

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Presenter's Biography

Dr. Xin Mao graduated in 2022 from the School of Chemistry and Physics at Queensland University of Technology (QUT), Australia. He then continued his postdoctoral research in the group of Prof. Aijun Du at QUT. In 2024, he joined the group of Prof. Yan Jiao as an ARC-funded research fellow at the University of Adelaide. His primary research interests include computational electrocatalysis, using molecular dynamics and constant potential models to study complex solid-liquid interface electrocatalytic reactions of small molecules.

Synthesis and Application Research on Conjugated Polyphthalocyanine—based Electrocatalytic materials

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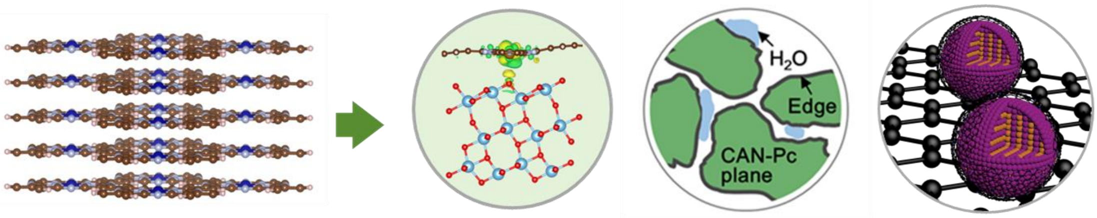
In recent years, the development of fuel cells has faced significant constraints due to the slow kinetics of cathode oxygen reduction reaction and the reliance on precious metal Pt based catalysts. Consequently, many researches have been focused on single–atom catalysts with adjustable electronic structures and unsaturated coordination. Among them, phthalocyanine has attracted widespread attention due to its strong structural design and uniform distribution of metal sites. The reporter initiated investigations from the atomic arrangement to adjust the surrounding environment of atomic sites, manipulate the spin state of active center, and enhance the synergistic strengthening of multi–scale active sites through various strategies including modifications of the cross-linking structure, heterogeneous coupling, and the expansion of derivative materials. These efforts have led to the optimization of the geometric and electronic structures of the materials, providing a theoretical foundation for the development of high performance electrocatalytic materials. These researches not only present new ideas for the design and application of single–atom electrocatalytic materials but also serve as references for translating theoretical advancements into practical applications for fuel cells.



Polyphthalocyanine Heterostructure Microenvironment Derived Material

Figure1. Polyphthalocyanine based electrocatalytic materials

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Di Yajing, a doctoral student at the School of Materials Science and Engineering, Beijing University of Chemical Technology, mainly researches the oxygen reduction catalyst performance of metal phthalocyanine based electrocatalytic materials and their derivatives. Simultaneously undertaking the theoretical calculations of the research group, exploring the charge transfer of adsorption states in catalytic material intermediates.

Molecular Modelling of Electrocatalyst Materials for Clean Energy Conversion

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The goal of achieving zero-carbon emissions by 2050 has driven the search for alternative solutions that can replace the traditional fossil fuel-based economy. With the technology and infrastructure in place to produce clean electricity from renewable sources such as solar or wind, the ability to generate it on a large scale is rapidly increasing. This presents a prime opportunity to produce carbon-free fuels and chemicals (for example, hydrogen) by electrocatalysis. The electrocatalysis method enables the conversion of green electricity into chemicals and fuels, and vice versa, providing a path towards a sustainable future.

One of the key challenges in electrocatalytic energy conversion reactions is the performance of the catalyst material. The need for electrocatalysts with high activity and selectivity is critical. Molecular modelling can play a significant role in designing these materials, especially when combined with experimental techniques. By gaining an in-depth understanding of electrochemical reactions through molecular modelling, we can propose new materials for various reactions. My presentation will briefly touch on how we have done this in the past and the challenges ahead. I will share my thoughts on how computational electrocatalysis will evolve in the future and the shift towards "Operando" modelling, and how machine learning might assist the progress. Additionally, I will present some of our recent works using machine learning to design materials that might have not existed before, and Operando modelling to uncover the potential and pH-dependent reaction mechanisms for electrochemical energy conversion reactions, and how that might aid us in designing better materials and reaction environments.

Presenter's Biography

Professor Yan Jiao obtained her PhD in Chemical Engineering from the University of Queensland in 2012. Since graduation, she has been working at University of Adelaide's School of Chemical Engineering. Yan is an ARC Future Fellow, a Young Tall Poppy, a Highly cited researcher, and one of 40 Rising Stars by The Australian. Yan's passion is to co-create a more sustainable world, using her expertise in molecular modelling and interdisciplinary collaboration spirit. Yan's expertise is the use of computational techniques for the design of clean and sustainable energy conversion materials. She has published more than 100 articles in leading journals such as Nat. Energy, Nat. ChemEng, Nat. Commun., J. Am. Chem. Soc., Angew. Chemie Int. Ed., and more. Her published works have received over 37,000 citations and with a h-index of 71. Yan has secured over one million Australian dollars in research funding as the Lead Chief Investigator. She is also a Chief Investigator and Program Leader for ARC Centre of Excellence for Carbon Science and Innovation.

Carbon-Based Catalyst to Accelerate Proton Spillover for Medical-level Electrosynthesis of H_2O_2 Disinfectant

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Abstract: Electrosynthesis of H_2O_2 has great potential for directly converting O_2 into disinfectant, although it is still a big challenge to develop effective electrocatalysts for medical-level production. Herein, we report the design and fabrication of electrocatalysts with biomimetic active centers, consisting of single atomic iron asymmetrically coordinated with both nitrogen and sulfur, dispersed on hierarchically porous carbon (Fe_{SA}-NS/C). The newly-developed Fe_{SA}-NS/C catalyst exhibited a high catalytic activity and selectivity for oxygen reduction to produce H_2O_2 at a high current of 100 mA cm^{-2} with a record high H_2O_2 selectivity of 90% and an accumulated H_2O_2 concentration of 5.8 wt.% sufficiently high for medical disinfection. Combined theoretical calculations and experimental characterizations verified the rationally-designed catalytic active center with the atomic Fe site stabilized by three-coordinated nitrogen atoms and one-sulfur atom ($Fe-N_3S-C$). It was further found that the replacement of one N atom in the classical $Fe-N_4-C$ active center with sulfur atom could induce an asymmetric charge distribution over N atoms surrounding the Fe reactive center to accelerate proton spillover for a rapid formation of the OOH* intermediate, thus speeding up the whole reaction kinetics of oxygen reduction for H_2O_2 electrosynthesis

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Presenter's Biography

Yan Li received her PhD degree from Zhejiang University in 2022. She joined UNSW Sydney in 2022 as a postdoctoral researcher under the supervision of Prof. Liming Dai in the School of Chemical Engineering. Her research interests focus on the design and synthesis of functional carbon-based nanostructures and their applications in electrochemical energy conversion and storage systems.

Structural design of carbon-based electrodes and catalytic reduction mechanism of carbon dioxide

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Effective reduction of CO_2 emissions and development of non-fossil fuel resources is crucial to reducing emissions of greenhouse gas CO_2 in the atmosphere and reducing our dependence on non-renewable energy resources. Using renewable energy to generate green electricity, the technology of producing highly value-added chemicals through electrochemical CO_2 reduction only needs to be carried out under normal temperature and pressure conditions, and has the advantages of fast reaction rate and high conversion efficiency. It has been subject to more and more research readers' attention in recent years. Although traditional bulk metal materials have certain catalytic activity for electrocatalytic CO_2 reduction reactions, they often have shortcomings such as high overpotential, low current density, poor product selectivity, and easy deactivation, which seriously hinder the use of bulk metal materials in electrocatalytic reactions, espeficaly in industrial applications in electrocatalytic CO_2 reduction. Compared with bulk metal materials, metal single-atom catalysts often exhibit unexpected catalytic activity in some important chemical reactions due to their unique electronic and geometric structures, special size effects and other characteristics. The project conducted systematic research on this issue, took the lead in proposing structural design principles based on key carbon-rich non-noble metal electrode materials in the high energy efficiency conversion process, and achieved a series of innovative research results.

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Presenter's Biography

Prof. Dr. Yang Hou is the winner of the National Outstanding Youth Fund, the "Hundred Talents Program" of Zhejiang University, the dean of the School of Biological and Chemical Engineering at the Ningbo Institute of Technology, the director of the Hydrogen Production Technology Research Center of the Zhejiang University Hydrogen Energy Research Institute, Royal Fellow of the Chemical Society, the Zhejiang Provincial High-Level Talent Program, the winner of the Zhejiang Provincial "Outstanding Youth" Fund, selected as a Global Highly Cited Scientist by Clarivate Analytics, Lu Jiaxi Excellent Mentor Award, Hou Debang Chemical Science and Technology Youth Award (1/1), China Petroleum and Chemical Industry Federation "Youth Science and Technology Outstanding Contribution Award" (1/1), China Chemical Industry Society Science and Technology Award (1/4), China Industry-University-Research Cooperation Innovation Award (1/1), China Petroleum and Chemical Industry Federation Science and Technology Award (1/5), etc.

Dr. Hou mainly engaged in research in the fields of carbon neutrality and green hydrogen. So far, more than 260 academic papers have been published in international journals such as Angew. Chem. Int. Ed., Energy Environ. Sci., Adv. Mater., Nat. Commun., etc. The papers have been cited more than 21,000 times, with an H-factor of 74. Dr. Hou served as a member of the Scientific Committee of the 17th Asia-Pacific Chemical Industry Alliance Conference. He has hosted the National Natural Science Foundation of China Outstanding Youth Fund Project, the National Natural Science Foundation of China-Region Key support projects of the Joint Fund for Innovation and Development, National Natural Science Foundation of China International (Regional) Cooperation and Exchange Projects, National Natural Science Foundation of China General Fund Projects, National Natural Science Foundation of China Youth Fund Projects, National Key R&D Program "Hydrogen Energy Technology" Key Special Subproject. Currently, Dr. Hou served as deputy editor: Nano-Micro Letters, deputy editor: Chemical Engineering Journal Advances, deputy editor: The Canadian Journal of Chemical Engineering, young communication expert: "Engineering", a journal of the Chinese Academy of Engineering, etc.

Computational Design of Sustainable 2D Semiconductors, Interfaces and Devices

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We introduce and review the recent advances on the computational design and modelling of two-dimensional (2D) semiconductor and heterostructures [1-4]. We show that the emerging monolayer family of MA_2Z_4 exhibits strong potential in electronics, optoelectronics, and deep ultraviolet (UV) applications. The design of Ohmic contacts to MA_2Z_4 monolayers with highly efficiency charge injection are discussed, which offers a route towards energy-efficient transistor applications. We then introduce the recent theoretical efforts in understanding the interfacial contact physics between semimetals (such as bismuth and antimony) with 2D transition metal dichalcogenide (TMDC) monolayers, which reveals antimony/TMDC as a promising metal/semiconductor material combination for achieving injection efficient Ohmic contact [1-3]. Finally, we introduce our recent efforts in the ab initio computational screening of sustainable 2D ultrawide bandgap (UWBG) composed of low human and environmental risks elements and demonstrate how such sustainable 2D UWBG materials can be employed to deliver low-leakage gate dielectrics, high-temperature transistor, and solar-blind UV photonic device applications [4]. These results shall provide a step forward towards the development of a more sustainable computing electronics landscape beyond the conventional silicon device technology.

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Presenter's Biography

Dr. Yee Sin Ang is an Assistant Professor at the Singapore University of Technology and Design (SUTD). He is a computational physicist, currently leading a research group working on the device physics and the computational design of 2D semiconductors, interfaces and nanodevices for future sustainable computing electronics. His research interests cover first-principles simulations of 2D materials and contact interfaces, theory of carrier transport, interfacial charge injection modeling, and the computational design of novel device architecture such as sub-10-nm transistors, spintronics, valleytronics, and brain-inspired devices. Dr. Ang received his PhD from the University of Wollongong, Australia (2014). Dr. Ang is the Associate Editor of *APL Electronic Devices*. He is one of the Emerging Leaders of the *Journal of Physics D: Applied Physics* (Class of 2022). He is listed among the World's Top 2% Scientists in the Applied Physics category by the Stanford University ranking since 2022.

From Fundamental Bio–Nano Interactions to Translational Nanomedicine

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Understanding the interactions of nanoengineered particles with specific proteins and cells is necessary to unlock their medicinal utility. Upon exposure to biological fluids, nanoparticles adsorb proteins, lipids and nucleic acids, resulting in the formation of a "biomolecular corona". This corona modulates downstream biological responses, including recognition by immune cells. Resolving the complexity of human plasma has been a major barrier to understanding the role of corona on biological response. We have previously engineered poly(ethylene glycol) (PEG) nanoparticles and investigated the formation of personalized biomolecular coronas on particles using plasma from a cohort of healthy donors and their impact on particle–immune cell interactions using an ex vivo human blood assay.[1] We demonstrated that the enrichment of immunoglobulins and complement proteins in biomolecular coronas is correlated with donor-specific nanoparticle association with human blood immune cells. We further demonstrated that the protein corona composition can be modulated by particle building blocks and protein pre-coatings.[2,3] Built on the previous works, we have recently studied the boost of poly(ethylene glycol) (PEG)-specific antibodies by SARS-CoV-2 mRNA lipid nanoparticle (LNP) vaccines.[4] After studying plasma samples from 130 adults, we discovered that anti-PEG antibodies were significantly boosted by mRNA-1273 vaccine and to a lower extent by BNT162b2 vaccines. Our study addresses timely and important questions regarding the anti-PEG antibody responses in healthy adults following SARS-CoV-2 mRNA-LNP vaccination and whether the induced anti-PEG antibody may impact the fate of other PEG-containing nanomedicines.[5] In this seminar, I will talk about our recent studies on the pharmacokinetics of mRNA lipid nanoparticle vaccine in humans and an ex vivo human leukemia blood model to assess the targeting of nanomedicine.

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Presenter's Biography

Yi (David) Ju is an ARC Discovery Early Career Researcher Award (DECRA) Fellow at RMIT University. His research interests include both fundamental bio–nano interaction studies (i.e., interactions between nanomaterials and the immune system) and translational research on developing novel nanoparticles for targeted drug and gene delivery. David's work has been pioneering in different aspects of materials science and nanotechnology. For example, his study has demonstrated that personalized biomolecular coronas can modulate nanoparticle–immune cell interactions in human blood (*ACS Nano 2020*) and that the mRNA lipid nanoparticle vaccines developed for SARS-CoV-2 can induce a polymer-specific antibody in human blood (*ACS Nano 2022* and *Nat. Rev. Immunol. 2023*). He has received several awards (e.g., *Victoria Fellowship*, *ACIS ECR lectureship, Most Significant CBNS Publication Award*) and secured $2 M ($1.3 M as a lead CI) in fellowship and research funding in the last 5 years. His research has led to 66 referred journal publications with >3400 Scopus citations and an average FWCI of 3.44. He currently serves as an Editor for the Journal of Materials Science and committee member of Victorian Branch of Royal Australian Chemical Institute (RACI).

Carbon-free ammonia combustion technologies for decarbonisation in high temperature manufacturing industries

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Manufacturing of ceramics, cements, glass and metal products requires high temperature processing, which is commonly achieved by combustion of fossil fuels, such as coal, oil and nature gas. High temperature manufacturing industries are under great pressures to reduce the carbon emission and move towards sustainable manufacturing. Combustion of carbon-free fuels, such as hydrogen (H_2) and ammonia (NH_3), can be an effective approach to reduce the carbon emission. Comparing to hydrogen, ammonia is more convenient in large scale transportation and storage, but more difficult to burn due to its high ignition energy, low combustion speed and narrow flammability range. In addition, the nitrogen in the molecule is a source of NOx emission in combustion. For large scale applications of ammonia fuel in high temperature industries, technology innovations are needed to achieve stable ignition and combustion as well as control of NOx emission. This talk reports our recent efforts in the development of ammonia combustion technology for manufacturing of ceramic tiles, which includes staged combustion burners, selective non-catalytic reduction (SNCR) and anhydrous ammonia selective catalytic reduction (SCR) techniques. Stable combustion of ammonia and desired temperature profile in ceramic kilns are achieved, both the amounts of NOx and residual ammonia emissions are well controlled to meet the regulatory standards, and the ceramic tiles fired with ammonia showed excellent properties.

Presenter's Biography

Yi-Bing Cheng is currently a Strategic Scientist at the Foshan Xianhu Laboratory, Guangdong Province and Professor of Wuhan University of Technology, China, and Emeritus Professor of Department of Materials Science and Engineering, Monash University, Australia. He is an elected Fellow of the Australian Academy of Technology and Engineering. He was an academic staff at Monash University between 1991 and 2018. He specialises in materials science and technology.. His current work at Foshan Xianhu Lab is to develop carbon-free fuel combustion technologies for high temperature manufacturing industries.

Sustainable Energy Storage Within Octahedral Molecule Sieves

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Tunnel-structured manganese dioxides (MnO_2), also known as octahedral molecule sieves (OMS), are widely studied in geochemistry, deionization, energy storage and (electro)catalysis. These functionalities originate from their characteristic sub-nanoscale tunnel framework, which, with a high degree of structural polymorphism and rich surface chemistry, can reversibly absorb and transport various ions. An intensive understanding of their structure–property relationship is prerequisite for functionality optimization, which has been recently approached by implementation of advanced (in situ) characterizations providing significant atomistic sciences. This presentation will thus timely cover recent advancements related to OMS and their energy storage applications [1-3], with a focus on the atomistic insights pioneered by researchers including our team: the origins of structural polymorphism and heterogeneity, the evolution of faceted OMS crystals and its effect on electrocatalysis, the ion transport/storage properties and their implication for processing OMS. These studies represent a clear rational behind recent endeavors investigating the historically applied OMS materials, the summary of which is expected to deepen the scientific understandings and guide material engineering for functionality control.

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Presenter's Biography

Yifei Yuan is now a professor at the College of Chemistry & Materials Engineering, Wenzhou University, China. He obtained his Ph.D. from Michigan Technological University and held a research assistant professor position at University of Illinois, jointly with Argonne National Laboratory. Yifei Yuan conducts research on fundamental studies of electrochemical energy storage materials. He investigates local atomic and nanometric structure-property correlations to elucidate design principles for advanced energy materials by rational syntheses, advanced microscopic characterization, and integration of material engineering strategies. His findings are published in journals like Nature Energy, Nature Sustainability, Nature Communications, etc., with a scholar H-index of 70. He was awarded Innovators 35 Under 35 (Asia Pacific, 《MIT Technology Review》2021). He also serves associated editor of the journal--《Carbon Energy》.

Heterogeneous Molecular Catalysis for Electrochemical CO_2 Reduction

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Electrochemical reduction of CO_2 (CO_2ERR) in aqueous electrolytes is one of the most promising routes for commercial CO_2 utilization. A switch from the currently used noble metal-based catalysts to the carbon-supported macrocyclic complexes could bring a much-needed cost reduction thus making the technology economically viable. However, the inherently low conductivity and a tendency of molecular catalysts to degrade during the long-term operation present a challenge for the catalyst design. We applied mechanistic investigations to tackle a challenging problem of the catalyst durability in CO_2ERR. It was determined that the loss of activity takes place due to the reductive carboxylation and co-occurring formation of inactive metal complex. Therefore, the stability could be greatly enhanced through the introduction of bulky donating substituents around the macrocyclic core. These insights allowed us to design and synthesise a catalyst bearing eight methoxy groups around the lateral aromatic moieties which demonstrates no noticeable degradation during the repetitive long run electrolyses. These design principles, combined with our recent development of bicarbonate electrolysis and heterogeneous molecular catalysts would provide a low-cost and very stable catalytic system for CO_2ERR.

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Biography: Dr Yijiao Jiang is a Professor at the School of Engineering at Macquarie University. She is the Co-Director of Macquarie Research Centre for Transforming Energy Markets and the Chief Investigator of ARC Industrial Transforming Research Hub for Smart Process Design and Control. After completing her PhD at University of Stuttgart, she worked as postdoc at ETH Zürich. She was then awarded UNSW Vice-Chancellor's Research Fellowship and ARC DECRA Fellow. Her research interests focus on transferring greenhouse gases and solid waste into clean fuels and high-value chemicals. She is an Associate Editor of Energy & Fuels and Carbon Catpure Science and Technology. She currently serves on the ARC College of Experts.

Nanocarbon and polymeric materials for green energy conversion and storage

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Green energy conversion and storage will eventually be one of the foundation for human being in terms of both energy need and environmental requirements. In this talk, we will highlight the progress of our recent studies in light to electricity conversion using organic photovoltaic and electricity energy storage using solid state lithium battery platform. Also, we will also make some proposals for the future perspertives in this regard.

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Presenter's Biography

Dr Yongsheng Chen, obtained his PhD from Univesity of Victoria in 1992, has been a Chair Professor at Nankai Universiy from 2002. His reseach focuses on green energy conversion (OPV) and storage (LIB) using nano carbon and poymeric materials.

He has published over 400 peer-reviewed papers including in Science and Nature and their sub-journals. These papers have generated over 80000 citing and he has been on the list of the most cited scientists from Clarivate for the last ten years with a H-index >120. He has also served as an editor/board member for Carbon, 2D Materials, Energy Storage Materials, Science China-Chemistry, Science China-Materials and etc.

Electrochemical Fischer-Tropsch Chemistry for Future Sustainable Fuels?

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Fischer-Tropsch (F-T) synthesis is a widely used industrial process for producing long-chain alkanes and alkenes, traditionally requiring thermal catalysts and syngas under high temperature and pressure. While effective, this conventional method is energy-intensive and less environmentally friendly. To address these challenges, an alternative approach using electrochemistry has emerged, leveraging the common surface species *CO and *H found in both thermal and electrochemical (EC) processes. This presentation will explore the concept of replicating F-T synthesis through electrochemical CO and CO_2 reduction—an area of research still in its infancy but with significant potential for improving production efficiency and sustainability. This talk will introduce EC F-T chemistry and offer insights into the challenges and potential future directions for achieving high-performance results.

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Presenter's Biography

Youngku Sohn, a Professor in the Department of Chemistry at Chungnam National University in South Korea, earned his PhD from the University of British Columbia, Canada, in 2004. He conducted postdoctoral research at the University of Texas at Austin (2005-2007) and the University of Waterloo, Canada (2007-2008). From 2008 to 2017, he was a faculty member at Yeungnam University. His research focuses on surface chemistry, particularly in areas such as electrocatalysis, photocatalysis, thermal catalysis, CO_2/CO energy conversion, water splitting, ammonia synthesis, and phosphor materials.

Heterogeneous Molecular Catalysts with Carbon Nanotube Substrates

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Carbon catalysts are promising precious-metal-free catalysts for various essential reactions. However, many carbon catalysts synthesized by high-temperature pyrolysis have inhomogeneous structures, making understanding and controlling their catalytic behaviors challenging. Our team has used carbon nanotube (CNT) substrates to produce heterogeneous molecular catalysts with well-defined structures to gain in-depth knowledge. First, we created coaxial 1D van der Waals heterostructures comprised of a CNT core and a thickness-tunable thienothiophene-pyrene covalent organic framework (COF) shell. The coaxial structure enables n-doping from the CNT core to the COF shell, controllable by varying COF shell thickness. The charge transfer from CNTs lowers COF's bandgap and work function, reducing the charge transfer barrier between the active catalytic sites and adsorbed oxygen intermediates and dramatically enhancing catalytic activity for oxygen redox reactions.[1] Second, we found that introducing β-substituents to Co porphyrins adsorbed on CNT substrates can synergistically modulate Co properties and catalytic activity. An octafluoro-substituted catalyst exhibited >94% H_2O_2 selectivity and a high turnover frequency of 3.51 per second at an overpotential of 200 millivolts in an acid electrolyte.[2] Third, we used Fe phthalocyanine anchored on CNTs as model Fe–N–C single atom catalysts to map their degradation. Detailed characterizations identified five degradation paths and revealed the beneficial role of electron-withdrawing substituents. The direct Fe leaching from Fe-N_4 sites plays a crucial role in early-stage degradation, which can be significantly suppressed by -F and -NO_2 substituents. The oxidative degradation became dominant with time, forming FeO_x nanoclusters on the CNT substrate, which the electron-withdrawing substituents can partially alleviate.[3]

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Presenter's Biography

Dr. Yuan Chen received a Bachelor's degree from Tsinghua University and a Ph.D. from Yale University. He was an Assistant and Associate Professor at Nanyang Technological University from 2005 to 2015. He has been a Professor at The University of Sydney since 2016. His research focuses on carbon materials and their sustainable energy and environmental applications, including batteries, supercapacitors, electrocatalysts, membranes, and antibacterial coatings. He received an ARC Professorial Future Fellowship in 2017 and an ARC Mid-Career Industry Fellowship in 2024. 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*. Visit our research group website: https://yuanchenlab.org/

Atomically thin 2D organic semiconductors

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Long-range and fast transport of coherent excitons is important for the development of high-speed excitonic circuits and quantum computing applications. However, most of these coherent excitons have only been observed in some low-dimensional semiconductors when coupled with cavities, as there are large inhomogeneous broadening and dephasing effects on the transport of excitons in their native states in materials. Here, by confining coherent excitons at the 2D quantum limit, we first observed molecular aggregation-enabled 'supertransport' of excitons in atomically thin two-dimensional (2D) organic semiconductors between coherent states, with a measured high effective exciton diffusion coefficient of ~346.9 cm^2/s at room temperature[1]. This value is one to several orders of magnitude higher than the values reported for other organic molecular aggregates and low-dimensional inorganic materials. Without coupling to any optical cavities, the monolayer pentacene sample, a very clean 2D quantum system (~1.2 nm thick) with high crystallinity (J-type aggregation) and minimal interfacial states, showed superradiant emission from Frenkel excitons, which was experimentally confirmed by the temperature-dependent photoluminescence (PL) emission, highly enhanced radiative decay rate, significantly narrowed PL peak width and strongly directional in-plane emission. The coherence in monolayer pentacene samples was observed to be delocalised over ~135 molecules, which is significantly larger than the values (a few molecules) observed for other organic thin films. In addition, the supertransport of excitons in monolayer pentacene samples showed highly anisotropic behaviour. Our results pave the way for the development of future high-speed excitonic circuits, fast OLEDs, and other optoelectronic devices[2,3].

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Presenter's Biography

Prof. Yuerui (Larry) Lu is a professor in the School of Engineering at the Australian National University (ANU). He received his Ph.D. degree from Cornell University in 2012, and B.S. degree from University of Science and Technology of China. Professor Lu is currently the chief investigator and program manager at the Australian Research Council Centre of Excellence for Quantum Computation and Communication Technology. His research interests include 2D quantum materials and optoelectronic devices, MEMS sensors and actuators, biomedical devices, etc. He has published 2 books (as editor), 7 book chapters, and more than 120 papers in high-impact journals, including Nature, Science, Nature Physics, etc. He was the recipient of several competitive awards, including the prestigious Prime Minister's Prizes for Science - the Malcolm McIntosh Prize for Physical Scientist of the Year in 2023, Pawsey Medal from Australian Academy of Science in 2023, etc.

Atomically dispersed electrocatalysts for highly efficient energy conversion reactions

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Keywords: single atom catalysts • atomic clusters • coordination environment • energy conversion reactions

Abstract:

The development of highly efficient catalysts to improve electrochemical performances is urgently needed due to the ever-increasing demand for energy conversion devices in the last few decades. Electrochemical water electrocatalysis and fuel cells are the two representatives for the next-generation energy conversion. However, the electrochemical performances are still not satisfying to be potentially used in industrial applications. Here we present our recent research on developing atomically dispersed electrocatalysts for energy conversion reactions.[1-5] We show that by carefully designing and tailoring the coordination environment, the efficiency of the applied catalysts could be maximized which would be highly beneficial for the electrochemical performances in their individual applications. For instance, *in-situ* exfoliated MXene coupled with Pt single atoms showed high hydrogen generation performance with a mass activity more than 40 times higher than the commercial Pt/C, while the epoxy-rich Fe single atoms boosted the oxygen reduction kinetics. All these provide theoretical and experimental guidance to develop highly efficient catalysts for energy conversion reactions in the future.

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Controllable synthesis, aggression structure and application of Graphdiyne

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Graphdiyne and its aggregate structure are an important direction in the current development of materials science. After ten years of research, the fundamental issues have been gradually solved, showing its application potential in many fields. In particular, the development of 1 and 2 dimension of graphdiyne aggregates and heterojunction materials, understanding their fundamental issues and potential applications in photo-electronics, energy, intelligent information and catalysis, represents the development trend of interdisciplinary. Based on the innovative concept, the self-assembly and self-organization methodology of graphdiyne based materials was established. Combined with the structure and controlled growth of carbon-based materials to controlled preparation of the aggregate structure from one dimension to two dimensions was realized. Because of its special electronic and chemical structure, graphdiyne has been widely concerned, and is forming a new research direction and field. It is a challenge and development trend in this field to explore the fundamental issues and potential applications of graphdiyne and its aggregate structure in the fields of energy, catalysis, photoelectronics, etc.

Presenter's Biography

Yuliang Li is a Professor at the Institute of Chemistry, Chinese Academy of Sciences，Professor, University of Chinese Academy of Sciences, Academician of the Chinese Academy of Sciences. Won the second prize of National Natural Science for three times in 2002, 2005 and 2014 respectively. Twice won the first prize of Beijing Science and Technology Award (Natural Science) and the second prize of Natural Science of Chinese Academy of Sciences. Won the first National Innovation Award in 2017, He Liang He Li Science and Technology Progress Award in 2017. Won the Outstanding Scientific and Technological Achievement Award of the Chinese Academy of Sciences in 2021. His research interests lie in the fields on chemistry of carbon and rich carbon, design and synthesis of low dimension and large size molecular aggregated structures based carbon and rich carbon materials with particular focus on the catalysis, energy, intelligent information and device integration.

Electrolysing CO_2 capture solution to CO on flame spray pyrolysis deposited silver

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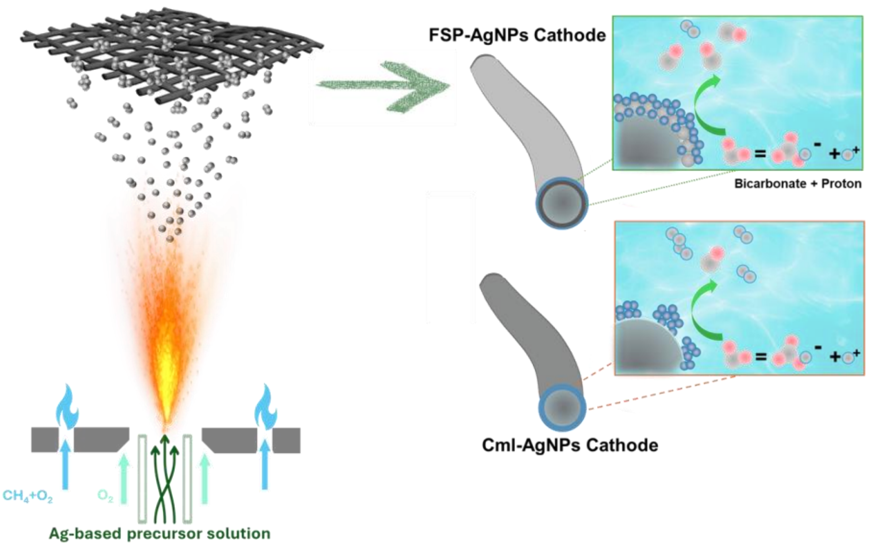
Carbon sequestration is crucial to mitigate the greenhouse effect through CO_2 capture and utilisation. Directly electrolysing CO_2 capture solution has emerged as a promising strategy to address the challenges associated with the gas-fed CO_2 electrolysis. Silver nanoparticles (AgNPs) are frequently used for bicarbonate electrolysis producing carbon monoxide. However, current loadings of AgNPs are unusually high. Hererin, we employ a cost-effective flame spray pyrolysis (FSP) to deposit AgNPs onto carbon cloth, prior to coating with commercial silver. A bicarbonate feedstock is then flow through the cathode within a flow-cell electrolyser for continuous CO production. The integration of FSP deposition and CO_2 electrolysis enables the system to achieve comparable CO selectivity while requiring only one-third of AgNPs loading compared to sole airbrushing deposition.



Presenter's Biography

Dr. Yuming Wu is a postdoctoral researcher at Macquarie University in Prof. Yijiao Jiang's team, specializing in CO_2 electrolysis, gas diffusion electrodes, and carbon materials. He earned his Ph.D. in Chemical Engineering from the University of Queensland, where he focused on mitigating electrolyte flooding in carbon-based gas diffusion electrodes for electrochemical CO_2 reduction. His current research extends to electrolytic system design and cathode development for bicarbonate electrolysis. Yuming has published 30 journal articles, accumulating over 1,000 citations.

Prof. Yijiao Jiang is the Deputy Director of Macquarie University Research Centre for Transforming Energy Markets, and Chief Investigator of ARC Industrial Transformation Research Hub (ITRH) for Smart Process Design and Control. *S*he has secured competitive external research grants from ARC DECRA Fellow, 3 ARC Discovery Projects, 1 ARC Linkage Project, and 2 ARC ITRHs with Rio Tinto, JITRI, EU H2020, CSIRO etc. She is an Associate Editor of *ACS Energy and Fuels* and *Carbon Capture Science and Technology* (Elsevier), She also serves on *the ARC College of Experts*.

TITLE: Defect formation, characterisation and design in functional materials

ABSTRACT

Ionic doping and/or substitution in solid-state materials provide opportunities to modify the materials for the peak performance and to create novel materials with new functions. In the past, the research in this field mainly focuses on the development of the relationship between the macroscopic structures (e.g. average structure determined by X-ray powder diffraction) and properties. It is found, however, that in many cases, such a relationship becomes very complicated and cannot be properly built. This is because that in a strongly correlated solid-state system, these ions can be structurally and/or chemically accommodated differently in local region but do not change the average structure. The trend that such ionic doping and/or substitution influence the properties is often not straightforward. In this talk, I will use several examples, including carbon materials, to demonstrate the local consequence of ionic doping and/or substitution and their impact on physical properties, and thus proposing new strategy to design the materials with high performance and new functions. I will also introduce a new characterisation methodology that can extend the micrometre-scale average structure towards multiple-length scales, including atomic-scale.

Bio:

Yun Liu is the Australian National University (ANU) Distinguished Professor and Australian Research Council (ARC) Georgina Sweet Australian Laureate Fellow, leading the Functional Materials Research group at the Research School of Chemistry (RSC), at the ANU.

Yun graduated from the Xian Jiaotong University, China with her BSc, MSc and PhD. She has since held five National Fellowship positions, including AIST and STA (now JSPS) Fellow at the National Institute of Advanced Industrial Science and Technology (AIST), Japan, and the ARC Queen Elisabeth II, Future Fellow and Georgina Sweet Australian Laureate Fellow in Australia. Her pioneering research focuses on defect chemistry, local structure and functional properties of condensed matters. She is internationally recognized for her application of complex materials chemistry to achieve novel functional properties for use in electronical technology, energy and environment. Her leading-edge research has led to ground-breaking research achievements, numerous innovation awards, large industry investments and considerable intellectual property outcomes, including 42 filed/issued patents and over 305 publications, including Nature, Science and Nature Materials.

She is the CI and program co-leader in the ARC Centre of Excellence for Carbon Science and Innovation.

MXenes from Discovery to the Modern Day and Beyond

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More than 40 stoichiometric MXene compositions and dozens of solid solutions and structures with various terminations have been reported since the first report on $Ti_3C_2T_x$ in 2011. The number of possible compositions is infinite if one considers solid solutions (more than 50 have been made in our lab) and combinations of surface terminations. New subfamilies of in- and out-of-plane ordered MXenes, oxycarbides, 2D borides, and silicides further expand the family of non-oxide 2D materials based on transition metals. MXenes have also opened an era of computationally driven atomistic design of 2D materials, and we are only starting our journey into the world of atomistically-designed materials. MXenes possess electronic, optical, mechanical, and electrochemical properties that differentiate them from other materials. MXenes are 2D building blocks for the assembled materials and devices that will power future technologies. Chemically tunable superconductivity has been demonstrated in Nb- and Mo-based MXenes. Highly nonlinear optical properties of MXenes are being explored. Several MXenes have been predicted to act as topological insulators. Many MXenes are metallic conductors but with a tunable density of states at the Fermi level, like in semiconductors. Moreover, their properties are tunable by design and can be modulated using an ionotronic approach, leading to breakthroughs in the fields ranging from optoelectronics and communication to energy storage, catalysis, sensing, and healthcare. In several applications, MXenes have already outperformed all other materials. In this talk, I'll discuss the progress in synthesis methods of MXenes, form original HF etching to CVD, and the effect of synthesis on composition and properties. I'll also outline prospects for applications of MXenes in fields ranging from electronics to healthcare, thermal management, communication, and energy generation and storage.

Yury Gogotsi is a Distinguished University Professor and Charles T. and Ruth M. Bach Endowed Chair in the Department of Materials Science and Engineering at Drexel University (Philadelphia, USA). He is the founding Director of the A.J. Drexel Nanomaterials Institute. Together with his students and colleagues, he made principal contributions to the development of materials for electrochemical energy storage and discovered MXenes. He is recognized as a Highly Cited Researcher in Materials Science and Chemistry and a Citations Laureate in Physics by Clarivate Analytics. He has received more than 60 awards for his research and teaching activities, including the Ceramic Prize from the World Academy of Ceramics, the MRS Medal, the Jan Czochralski Award from the European MRS, the ACS Award in the Chemistry of Materials, the Friendship Award from P.R. China, etc. He is a Fellow of the National Academy of Inventors, the World Academy of Ceramics, the European Academy of Sciences (EurASc), Academia Europaea, and many professional societies. He holds honorary doctorates from several European Universities.

Unveiling Catalyst Engineering Strategies in Steering Urea Electrooxidation Selectivity

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Recent advancements in the electrochemical urea oxidation reaction (UOR) present promising avenues for wastewater remediation and energy recovery. Despite progress toward optimized efficiency, hurdles persist in steering oxidation products away from environmentally unfriendly products, mostly due to a lack of understanding of structure-selectivity relationships. In this study, the UOR performance of Ni and Cu double hydroxides, which show marked differences in their reactivity and selectivity is evaluated. CuCo hydroxides predominantly produce N_2, reaching a current density of 20 mA cmgeo^{-2} at 1.04 V – 250 mV less than NiCo hydroxides that generate nitrogen oxides. A collection of in-situ spectroscopies and scattering experiments reveal a unique in situ generated $Cu^{(2-x)+}$-$OO^{-\bullet}$ active sites in CuCo, which initiates nucleophilic substitution of NH2 from the amide, leading to N-N coupling between *NH on Co and Cu. In contrast, the formation of nitrogen oxides on NiCo is primarily attributed to the presence of high-valence Ni^{3+} and Ni^{4+}, which facilitates N-H activation. This process, in conjunction with the excessive accumulation of OH^- ions on Jahn-Teller (JT) distorted Co sites, leads to the generation of NO_2^- as the primary product. This work underscores the importance of catalyst composition and structural engineering in tailoring innocuous UOR products.

Presenter's Biography

Yuwei Yang is currently a postdoctoral researcher at the Centre of Excellence in Carbon Science and Innovation and School of Chemical, the University of New South Wales, Australia. Her current research interests focus on advanced nanomaterials for electrochemical renewable energy technologies, and establishing structure/ function relationships for functional nanoscale materials and interfaces using synchrotron radiation methods.

Electrocatalysts design for High Energy Metal-Carbon Dioxide Batteries

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Severe global warming has resulted in pledges by current society to achieve the goals of carbon neutrality with projections of atmospheric carbon peaking followed by eventual falls. In this context, how to achieve eco-efficient and environmentally sustainable CO_2 capture, and to reconstruct energy device systems for balancing reduction of carbon emissions and growing energy demands has become a worldwide challenge. Rechargeable metal–CO_2 batteries are considered potential candidates for advanced energy storage devices and CO_2 fixation.

In this talk, I will report our recent progress in metal-CO_2 batteries. Specifically, I will introduce the K–CO_2 battery with a carbon-based metal-free electrocatalyst, exhibiting a higher theoretical discharge potential compared to Na–CO_2 batteries and demonstrating exceptional cycling stability[1]. Furthermore, I will highlight our research on the synthesis and characterization of NiFeCoCuRu high-entropy alloys (HEAs) with nanoscale dimensions. These HEAs, when loaded onto a carbon matrix, significantly enhance the efficiency of lithium-mediated CO_2 redox reactions, exhibiting a low overpotential and exceptional durability exceeding 2900 hours[2]. Additionally, our investigation also reveals the catalytic effects of C-N species within solid electrolyte interphase (SEI) layers in Li-CO_2 batteries. These C-N species facilitate accelerated kinetics for the formation and decomposition of Li_2CO_3 by establishing a bidirectional fast-reacting bridge for carbon dioxide reduction and evolution reactions (CRR/CER). Leveraging this insight, we have developed a strategy to design a C-N rich SEI via dual-salt electrolytes, leading to substantial improvements in the cycle life of Li-CO_2 batteries[3-5].

These advancements underscore the potential of tailored electrocatalysts and innovative electrolyte design to address critical challenges in high-energy metal-CO_2 batteries, paving the way for next-generation energy storage solutions.

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Presenter's Biography
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Professor Zaiping Guo is an Australian Laureate Fellow at School of Chemical Engineering, The University of Adelaide. She is also an Associate Editor for Chemical Science, a flagship journal of the RSC. She was elected to the Fellow of Australian Academy of Science and Australian Academy of Technological Sciences and Engineering in 2023. Her research focuses on the design and application of electrode materials and electrolyte for energy storage and conversion, including rechargeable batteries, hydrogen storage, and fuel cells. Her research achievements have been recognized through numerous awards, including an ARC Queen Elizabeth II Fellowship in 2010, an ARC Future Professorial Fellowship in 2015, an ARC Laureate Fellowship (2021), and the Clarivate Analytics Highly Cited Researcher Award in 2018, 2019, 2020, 2021, 2022, and 2023. She was also awarded 2020 NSW Premier's Prizes for Science & Engineering for Excellence in Engineering or Information and Communications Technology.

In-situ Integration of 2D g-C_3N_4 into Oriented MOF Films

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Two-dimensional (2D) materials, such as graphitic carbon nitride (g-C_3N_4), have attracted significant attention due to their high surface area, tunable electronic properties, and excellent potential in photocatalysis and energy storage applications.[1] However, challenges such as limited charge separation and poor conductivity often hinder their practical performance.[2] Metal-organic frameworks (MOFs), with their highly ordered porous structures and tunability, provide an ideal platform for incorporating 2D materials, potentially enhancing their catalytic and electronic capabilities.[3, 4] Despite these advantages, many current approaches primarily rely on simplistic and disordered mixing of g-C_3N_4 and MOF powders, which often leads to weak interfacial contact and random distribution of active sites, ultimately hampering charge transfer and reducing the efficiency of the hybrid materials.[5, 6]

To improve charge separation, enhance transfer efficiency, and optimize the utilization of active sites, we developed a strategy for the orderly assembly of g-C_3N_4 and MOFs. In this work, we employed a highly oriented and structured MOF film as a precursor, followed by the in-situ synthesis of g-C_3N_4 within the MOF pore system. By optimizing experimental conditions, we successfully preserved the structural integrity and properties of both the MOF and g-C_3N_4. The X-ray diffraction (XRD) pattern revealed a characteristic (002) diffraction peak for g-C_3N_4 at 27.5°, corresponding to the periodic stacking of adjacent planes in its layered structure. Simultaneously, scanning electron microscopy (SEM) images further demonstrated the uniform distribution of g-C_3N_4 nanosheets within the MOF channels. Our approach addresses the limitations of weak interactions and inconsistent distribution commonly found in conventional mixture techniques. This strategy opens new opportunities for enhancing photocatalytic processes, such as CO_2 reduction and H_2 production, as well as improving energy storage technologies like supercapacitors.

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Zejun Zhang obtained his PhD in Chemistry in 2022 from the Karlsruhe Institute of Technology, Germany, where he conducted research on the application and tunable properties of photoswitchable surface-mounted metal-organic frameworks, under the supervision of Prof. Christof Wöll and Prof. Lars Heinke. Currently, he is a postdoctoral researcher in Functional Materials Research Group at the Australian National University. His research interests primarily focus on the fabrication and application of 2D and 3D carbon scaffolds for catalysis and sensing, the preparation, structure, and properties of polar functional materials, as well as energy storage materials.

Stable Anode for Efficient Zinc Metal Batteries

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Rechargeable zinc metal batteries (RZMBs) have been scrutinized as a promising energy storage technology whose full potential largely relies on stable Zn anodes. In this talk, I will showcase our recent advances in rationalizing stable Zn anodes for efficient RZMBs. We identified the prevalent soft-short issue hidden in Zn anode stability assessments and proposed pertinent reliable testing protocols for genuine evaluation. Our research also revealed that Zn^{2+} transport within solid-electrolyte interphases is the rate-determining step for in-cell carrier transfer kinetics in intercalation-type RZMBs, and elaborated interphase chemistries to enable practical pouch cells with high device-level specific energy and excellent durability. Moreover, we developed advanced gel electrolytes with enhanced interfacial chemistries for stable Zn anodes, along with high areal-capacity flexible RZMB porotypes demonstrated.

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Presenter's Biography

Dr. Zengxia Pei is a Lecturer and Horizon Fellow at the University of Sydney (USYD). He received his PhD in 2017 from City University of Hong Kong. He joined USYD in 2018 as a Vice-Chancellor's Research Fellow, and later he secured the ARC DECRA Fellowship in 2019. Dr. Pei works on nanomaterials for sustainable energy storage and conversion, with special interests in aqueous batteries, polymer electrolytes, as well as electrocatalysis. He has been consecutively recognized as a Global Highly Cited Researher (Top 1%) in 2020-2023, and was named the Australian Research Top Rising Star (1 out of 5 in Chemical/Material Science) from 2019 to 2021. Dr. Pei was also awarded the USYD Vice-Chancellor's Award for Excellent Early Career Researcher in 2023.

Biorefining of Agricultural Biomass into Sustainable Functional Materials

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Agricultural biomass, such as sugarcane bagasse and rice husk, is an abundant renewable bioresource for producing sustainable products. It has been extensively studied for producing fuels and chemicals. However, high production cost and low product value have hindered its commercialisation. Biorefining of agricultural biomass into high-value functional materials have the potential to significantly improve process economics.

Professor Zhanying Zhang and his team at Queensland University of Technology (QUT) have been at the forefront of developing such advanced biorefinery technologies. They initially developed pretreatment technologies for the efficient production of fermentable sugars from sugarcane fibers, from which biofuels and biochemicals were synthesised through microbial fermentation (1,2). In recent years, Professor Zhang and his group have been utilising the biomass pretreatment and fractionation technologies as a platform technology for producing advanced functional materials for various applications. Recent activities include tailored production of lignin-containing nanocellulose (3), photonic films derived from cellulose nanocrystals for solvent detection and radiative cooling, hard carbon derived from lignin for sodium ion batteries, and nanosilica derived from rice husks for rubber and polymer composites applications. In this presentation, Prof Zhanying Zhang will summarise their recent achievements in these areas.

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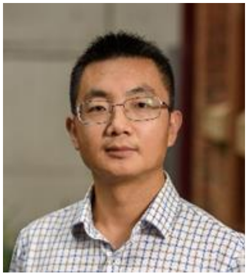
Biography

Dr Zhanying Zhang is a professor of Bioprocess Engineering at QUT. His research focuses on the high-value utilisation of agricultural biomass. Prof Zhang previously developed several patented biomass pretreatment technologies for producing fermentable sugars and subsequently biofuels and biochemicals through microbial fermentation. His current research interests focus on the production of biomass-derived functional materials for energy storage and management applications, and biomass-derived functional food ingredients for human health improvement. His ongoing research projects include lignin-derived hard carbon for battery anode applications, CNC-derived photonic films for radiative cooling, rice husk-derived biosilica for rubber and polymer composites, and functional food ingredients from brewer's spent grain and grape pomace.



Enhanced carbon dioxide conversion using graphene-based catalysts

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Converting carbon dioxide into valuable fuels and chemicals are critical for decarbonisation and clean energy transition. In the electrochemical route, the performance of carbon dioxide conversion (efficiency, selectivity, and stability) is primarily determined by the catalysts. In this talk, I will present several strategies to optimise the structure and properties of graphene-based catalysts to achieve enhanced carbon dioxide conversion, including: (i) metal halide perovskite $CsPbI_3$ stabilized by reduced graphene oxide (rGO) to exhibit >92% Faradaic efficiency toward formate production [1]; (ii) well-dispersed $Cu@CuO_x$ nanoparticles supported on Ar-plasma treated 3D vertical graphene (VG-Ar) to achieve a high portion of liquid products, i.e., formate, ethanol, and n-propanol [2]; and (iii) Cu nanoparticles anchored on VG to be reconstructed by a reduction-oxidation-reduction (ROR) electrochemical treatment for tunable pathways between intermediates *COOH- and *OCHO-derived products [3]. These findings show graphene as a promising material to rationally design and engineer robust catalysts for transforming carbon dioxide toward valuable fuels and products.

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Presenter's Biography

A/Prof. Zhaojun Han received his PhD degree in Electrical and Electronic Engineering from Nanyang Technological University, Singapore. His current research focuses on developing low-dimensional functional materials to tackle the challenges in materials, energy and environmental science. He is the recipient of several awards including ARC Future Fellowship, Julius Career Award, and Discovery Early-Career Researcher Award (DECRA).

Cross-scale Modelling for Dynamic Ionic Systems in Graphene Membrane Energy Storage Devices

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Dynamic ionic systems confined inside nanoporous electrodes are the hidden engine of various electrochemical energy storage and conversion technologies. Under dynamic working conditions, the ionic systems are driven far from equilibrium. The interplay of multiple ion transport processes in the heterogeneous electrodes 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 in electrified nanoporous materials are essential to developing new systems and optimising existing ones for these energy technologies. However, the spatiotemporal evolution of ions/electrons is poorly understood, a crucial bottleneck to bridging fundamental science with engineering applications. Dynamic models crossing multiple time and length scales are urgently needed to digitalise the ion/electron spatiotemporal evolutions in the nanoporous electrodes for optimal design, accurate diagnosis, and optimal operation in engineering applications. In this talk, I will review my group's recent progress in the cross-scale modelling of ion dynamics in graphene membrane-based energy storage devices, including atomistic simulations for nanoscale interface ionic structures/properties, nanoscience-based continuum models and physics-based equivalent circuit models for mesoscale ion dynamics, and machine learning approaches for macroscopic device designs. I will use several examples to demonstrate how these cross-scale digital models enable the critical, in-depth understanding of the nanoconfined dynamic ionic systems and drastically enhance the performance via rational design.

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 his Bachelor's and Master's degrees in Engineering Mechanics at Tsinghua University in China. He got a Ph.D. in Materials Science and Engineering 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 is 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.

Phthalocyanine–based materials for electrocatalysis

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Applications of phthalocyanines (Pcs) in electrocatalysis—including the oxygen reduction reaction (ORR), the carbon dioxide reduction reaction (CO_2RR), the oxygen evolution reaction (OER), and the hydrogen evolution reaction (HER)—have attracted considerable attention recently. The basic Pc macrocycle is a rigid structure consisting of four isoindole subunits attached via meso-positioned nitrogen atoms, which allows diverse functionalities by variation of the central ion, the ligands bound at the axial positions of the metal center, and the substituents at the peripheral and non–peripheralpositions of the Pc back bone. This report focuses on the molecular design, carriers control, and electrodes applications to improve the catalytic performance of Pcs. This report will also discuss the structure/composition–catalytic activity relationships for Pcs and its derivates. It provides guidance for a scalable and cost–effective approach for other atomic site electrocatalysts.

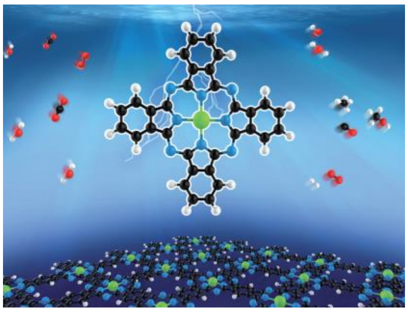

Fig. 1. Schematic diagram of phthalocyanine molecular structure

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Zhang Zhengping, a professor at Beijing University of Chemical Technology, was awarded the National Excellent Youth Science Fund in 2021. He mainly engaged in the electrocatalytic materials and catalytic electrodes in field of hydrogen energy and environment. Prof. Zhang has published more than 80 papers in international academic journals, including *Chem. Soc. Rev.*, *J. Am. Chem. Soc.*, *Adv. Mater.*,and *Angew. Chem. Int. Ed.*

Boron-based materials: Energy conversation and storage

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Boron, carbon, nitrogen and hydrogen together forms many compounds (denoted as $BCNH_x$) that have high hydrogen capacity (weight percent). These compounds typically feature extensive intra- and/or intermolecular $N{-}H^{\delta+}$---$H^{\delta-}{-}B$ dihydrogen interactions, which enable facile dehydrogenation. By adjusting the number and relative atomic positions of B, C, N and H, we have been able to tune the physical and chemical properties of $BCNH_x$. In this talk, I will present some of our recent reports on novel synthesis methods and exploring new $BCNH_x$ compounds for hydrogen storage, which has been one of the bottlenecks for the development of hydrogen economy. By guiding the dehydrogenation, $BCNH_x$ compounds can be converted to nanomaterials with interesting applications in energy harvest, catalysis, photothermal evaporation. Boron and nitrogen together form a layered compound, hexagonal boron nitride (h-BN), which is isostructural to graphene. h-BN nanosheets could be an excellent atomically thin protective layer over Cu substrate if it is made with high quality. We found boron nitride nanosheets dramatically improve the thermal response of temperature-sensitive hydrogels. h-BN nanosheets have recently been found to show interesting catalytic properties such as selective oxidative dehydrogenation of alkane to alkene and photocatalytic H_2 and O_2 generation from water.

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Presenter's Biography

Professor Huang heads a team of cross-disciplinary experts working on the Hydrogen Energy Program at UTS, which aims to develop key hydrogen technologies and prepare skilled workers for the emerging global hydrogen economy. Zhenguo's research has centered on boron chemistry for energy conversion and storage, and his wider research interests are in the fields of hydrogen storage materials, electrolytes, and two-dimensional boron-containing nanosheets. His breakthrough in hydrogen storage and Na-ion batteries has been successfully commercialized in partnership with Melbourne-based specialist chemical manufacturer, Boron Molecular. Zhenguo has been awarded an ARC DECRA and ARC Future Fellowship. He is a Research Advisor at the National Institute for Materials Science in Japan and a recipient of the Humboldt Research Fellowship for Experienced Researchers (Alexander von Humboldt Foundation). He is the Chair of the International Hydrogen Carriers Alliance. He received a University of Wollongong Vice-Chancellor's Award for Outstanding Achievement in Research Commercialisation, Impact and Engagement, and the UTS Vice-Chancellor's Awards for Research Excellence: Research Leadership and

Development Award. Zhenguo is a graduate of the Australian Institute of Company Directors. He received his PhD at the UOW (2007), followed by a postdoctoral appointment at The Ohio State University in the US.

High-Quality Atomically Thin Superconductors

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I will present our fabrication of high-quality atomically thin superconductors and heterostructures, which include conventional superconductors (Pb, Ga, etc.), iron-based superconductors (FeSe, $FeSe_{1-x}Te_x$, KFeSe, etc), copper-based superconductor $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi2212)-Bi_2Se_3 heterostructures. Their exotic physics will be briefly discussed. I will showcase our fabrication techniques and highlight the unique physics exhibited by these materials. The discussion will provide a concise overview of the intriguing properties displayed by these atomically thin superconductors and heterostructures. Their exotic behaviors hold tremendous potential for advancing fundamental understanding and exploring practical applications in the realm of superconductivity.

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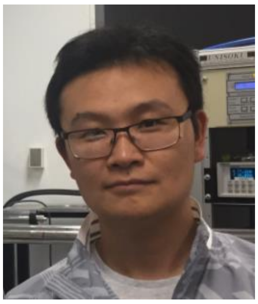
Presenter's Biography



I am a Scientia Senior Lecturer and ARC Future Fellow at the University of New South Wales, specializing in quantum materials. My research focuses on exploring topological insulators, interface superconductors, and two-dimensional materials. I am dedicated to advancing our understanding of quantum materials and inspiring future scientists. In my work, I employ cutting-edge techniques like molecular beam epitaxy (MBE) and scanning tunneling microscopy (STM) to investigate these materials at an atomic scale, uncovering their unique properties and potential applications. My goal is to contribute to the growth of this captivating field and make meaningful contributions to the world of quantum materials research.

Carbon-based Hybrid Energy Materials

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The practical application and promotion of carbon-based hybrid materials are severely restricted in the fields of energy and environment due to the poor controllability of surface/interface structure and low charge transfer efficiency. The reporter has carried out systematic studies on the regulation of interface structure and charge transfer characteristics of carbon-based hybrid materials, and have achieved the following progress: Precise regulation of the atomic arrangement at the interface of carbon-based hybrid materials was achieved by domain limited pyrolysis, revealing the relationship between the interface structure and electrochemical activity, and providing a new strategy for the surface interface regulation of carbon-based hybrid materials; A new strategy of salt template-induced conjugated bonding of interfacial atoms was developed, and controllable construction of carbon-based hybrid materials with three-dimensional regular polar pore structure was realized, which provides a new idea for reducing the activation energy of reactants; The surface-heterogeneity strategy of carbon-based hybrid materials was proposed, and multi-level coupling interfaces with abundant active sites are constructed, which lays a foundation for improving the interface charge transfer efficiency.

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Presenter's Biography

Zhihong Tian is a Yellow River Scholar and professor at Henan University. She obtained her first Ph.D. degree in engineering at Zhengzhou University in 2018, and a second Ph.D. degree in natural science at Max Planck Institute of Colloids and Interfaces/Potsdam University in 2019 in Germany. After finishing her Ph.D. studies, she worked as a postdoctor in Professor Markus Antonietti's group at Max Planck Institute of Colloids and Interfaces in Germany. In January 2021, she joined the Engineering Research Center for Nanomaterials at Henan University. Her research interests are on the structural design and performance optimization of porous carbon materials. Current effort in her group is directed towards constructing carbon skeletons at atomic and molecular level, functionalizing the carbon materials through surface modification, pore structure design and active sites tailoring, and investigating their gas adsorption, energy storage, and catalytic properties. She has published more than 40 scientific papers in the above research fields, including Angew. Chem. Int. Edit., Adv. Mater., Adv. Energy Mater. et al. She has presided over 2 projects of National Natural Science Foundation of China, an overseas project funded by China Scholarship Council, a project of Henan Center for Outstanding Overseas Scientists and obtained four authorized national invention patents.

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 researches based on ferroelectric photoelectrode $BiFeO_3$ show that these intrinsic dipoles can also be tunned via external poling treatment, wherein the aligned dipole moment can lead to precisely control of the band bending degree, leading to adjustable charge separation and transfer efficiency in the ferroelectric $BiFeO_3$ 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 Future 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.

Pyrolysis-Free Covalent Organic Polymers Directly for Oxygen Electrocatalysis

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Highly efficient electrocatalysts are vital to meet the energy and environmental challenges. Although numerous nonprecious-metal or metal-free carbon-based catalysts have been demonstrated to entirely or partially replace noble-metal-based electrocatalysis, the absence of precise design and predictable process hindered the development. Covalent organic polymers (COPs) are a class of molecular geometric constructs linked by irreversible kinetic covalent bonds through reticular chemistry. Unique structural tailorability, diverse design principles, and inherent well-defined construction in pristine COPs naturally provide a great platform to study the structure−property relationship of active sites and exhibit unique features for application. Furthermore, we discuss the possible future directions on designed synthesis of intrinsic COPs without carbonization to modulate active sites and the density of active sites at the molecular level. COP materials as a new family of electrocatalysts offer practical possibilities to study the structure, mechanism and kinetics of energy electrocatalysis and may lead to a better solution for energy and environmental issues.

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Presenter's Biography

Zhonghua Xiang is a professor and director of the Molecular Energy Materials R&D Center at Beijing University of Chemical Technology (BUCT). He received his B.S. in Xiangtan University in 2007, Ph.D. in 2013 at BUCT and was a postdoctoral researcher at Case Western Reserve University (2013–2014). His research interests are focused on the design and synthesis of molecular energy materials, mainly including covalent–organic frameworks for fuel cells and flow battery. He has published over 110 SCI articles in *Acc. Chem. Res.*, *J. Am. Chem. Soc., Angew. Chem. Int. Ed., Sci. Adv., Nat. Commun., Adv. Mater.* et al., and authorized 19 invention patents, 6 of which have been successfully transferred to the enterprise; He led and presided over the National Key Research and Development Program of China, the key international cooperation projects of the National Fund Commission, National Science Fund for Outstanding Young Scholars, Beijing National Science Fund for Distinguished Young Scholars, PetroChina and other enterprises; He won the First Prize (Natural Science) of Scientific and Technical Awards of Ministry of Education of China as a second winner; the Hou Debang Chemical Science and Technology Award for young scientists; the China Renewable Energy Society Excellent Science and Technology Talent Award; He was an associate board members of Next Mater., and young board members of Green Chem. Eng., eScience, Chinese Chem. Lett. He was appointed as the Deputy Director of the Youth Working Committee of China Renewable Energy Society, member of the Hydrogen Energy Professional Committee of China Renewable Energy Society, and member of the International Academic Exchange Working Committee of China Chemical Society.

Metal-Free Carbon Catalysts for Catalytic Cancer Therapy

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Nanoparticle-based catalysts have been developed for catalytic nanomedicine towards safe and effective treatment of diseases. Nanomaterial innovation plays a key role in driving progress of the field. In this talk, I will present our recent research progress on development of bioresponsive metal-free carbon catalysts for chemodynamic and photodynamic therapy by leveraging the internal or external stimuli-triggered catalytic reactions of metal-free carbon catalysts. Defect-rich graphene quantum dots (GQDs) were developed for efficient reactive oxygen species (ROS) generation, particularly in the H2O2-rich tumor microenvironment to cause multi-level damage of subcellular components. While a desirable anti-cancer performance was achieved, the catalytic performance was found to strongly depend on the defect density. It is for the first time that the defect-induced catalytic generation of ROS by metal-free carbon catalysts in the tumor microenvironment was demonstrated and the associated catalytic mechanism was elucidated. Built on these findings, a metal-free carbon co-catalyst consisting phosphorus-doped carbon nitride (P-C_3N_4) and defect-rich GQDs, was developed for enhanced chemo-photocatalytic cancer therapy. This study demonstrates, for the first time, a cancer therapeutic of GQD/P-C_3N_4 composite that utilizes a two-step cascade effect using initially NIR-triggered GQD nanoparticles to activate P-C_3N_4 to photocatalytically generate ROS for effective and targeted cancer therapy.

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Presenter's Biography

Zi (Sophia) Gu is an Associate Professor at the School of Chemical Engineering, University of New South Wales (UNSW Sydney). She leads a NanoBiotechnology Research Group at UNSW, and is a member in Australian Centre for NanoMedicine and UNSW RNA Institute. After PhD training at the University of Queensland and Cornell University, she secured a NHMRC Fellowship and joined UNSW in 2016. Her research focuses on developing advanced nanomaterials and delivery strategies to address critical issues in medicine and health. To date, she has published over 90 journal papers in the area of nanomaterials and nanomedicine. She is an Editor-in-Chief of Cancer Nanotechnology and Associate editor of Journal of Nanobiotechnology and Exploration.

2D metal oxide nanostructures for green hydrogen production

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Hydrogen energy has been regarded as one promising alternative to displace current fossil energy resources by its high energy value and zero CO_2 emission to address the increasing environment and energy crises. Especially, electrochemical water splitting hydrogen production is expected to be the most feasible approach with a good balance of cost and efficiency, in which electrocatalysts are the most critical component and govern the conversion cost and energy consumption. Therefore, the search of affordable catalysts with comparable catalytic performance to replace with the current expensive noble-metal-based catalysts in real water conditions is an urgent priority. In this presentation, inspired by the salient properties of 2D materials, promising 2D metal oxide-based electrocatalysts for electrochemical hydrogen production through mechanism understandings and performance upgrades will be presented. It is expected that this presentation will provide some insights in designing low-cost but efficient non-noble-metal catalysts for reaching affordable green hydrogen energy

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Our advances in rational design of perovskite materials for energy storage and conversion

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Abstract

ABX_3-tye Perovskite material has attracted considerable attention as a key functional material for energy storage and conversion device, like solar cells, fuel cells, electrolysis cells, and lithium ion batteries and supercapacitors. The advantages of perovskites are from their versatibility of their compositions with more than 90% of the element in the Periodic Table of Elements can be doped into the perovskite lattice structure. We have conducted the research in the development o perovskite materials for various applications for around 30 years. In this research, we will mainly discuss our advances in the perovskite materials for various energy-related applications, from solar cell to fuel cells to batteries and water electrolysis. The rational design is focused.

Presenter's Biography

Zongping Shao is a John Curtin Distinguished Professor at Curtin University, Australia. He obtained his Ph.D. from the Dalian Institute of Chemical Physics, China, in 2000. He worked as a Visiting Scholar at the Institut de Researches sur la Catalyse, CNRS, France and as a Postdoctoral Research Fellow at the California Institute of Technology, USA, from 2000 to 2005. He got ARC future fellowship in 2010, and relocated to Curtin University in 2012.Since 1995, he started the research on perovskite materials. His main research is new energy materials and devices, from both fundamental research to applications, including fuel cells, batteries, solar cells, and electrolysis cells. Up to now, he has published around 900 journal papers, including 5 in Nature, 1 in Science, 2 in Nature Energy, 1 in Nature Catalysis, and 15 nin Nature Communications. The papers have attracted more than 78,000 citations. He is Clarivate highly cited researcher in both fields of Chemistry and Materials Science.

Catalytic Revaluation of Carbon-Based Molecules

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The revaluation of carbon-based molecules holds immense potential in addressing both energy demands and environmental concerns, particularly the reduction of greenhouse gases such as carbon dioxide. Methanol, a versatile carbon compound, can be reformed through oxidation and reduction processes, leading to the production of hydrogen and valuable organic molecules without releasing CO_2. By employing various catalysts, our research demonstrates how methanol can undergo selective reformation, with the dual benefits of hydrogen generation and organic synthesis. Additionally, the reduction of carbon dioxide plays a crucial role in mitigating global warming. In this study, we explore catalytic CO_2 reduction pathways that yield products such as carbon monoxide, methane, and formaldehyde, offering new routes for carbon utilization. Our results highlight the influence of catalyst choice on product selectivity and efficiency, further advancing the revaluation of carbon molecules. From our work, the role of nanocatalysis and multi-modal catalysis, including photocatalysis, electrocatalysis, and photoelectrocatalysis, promises widespread applications in carbon conversion and sustainable energy solutions. These approaches open new frontiers for carbon revaluation in a rapidly evolving energy landscape.

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Biography Dr. Zongyou Yin obtained his B.S. and M.S. degrees at Jilin University in China, and completed his Ph.D. at Nanyang Technological University (NTU) in Singapore. Then, he started his postdoc careers at NTU/Singapore, IMRE/Singapore, followed by MIT and then Harvard University. Dr Yin started his own Research Group at Australian National Univesrity (ANU) from 2017. His group's research is interdisciplinary, encompassing AI-driven materials innovations, nano-to-atomic materials science, fundamental relationship among materials-structures-devices, and synergistic integration of multi-functions towards systems for renewable energy and wearables applications.

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