



ABSTRACT BOOK

International Conference on
**Materials for
Green Future**

March 25-28, 2024

JW Marriott Phuket Resort & Spa
Phuket, Thailand

A central graphic featuring a globe made of a blue wireframe mesh. Surrounding the globe are various icons representing sustainability and technology: a sun, a recycling symbol, a water drop, a leaf, a wind turbine, and a document with a checklist. The background is a dark blue gradient with faint, glowing geometric shapes.

Exhibitor

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A logo for "Sustainable Materials and Technologies" featuring a green recycling symbol and the text "Sustainable Materials and Technologies" above it.
Next

<https://greenmaterialsconference.com>

17:00 - 21:00 Welcome Reception

@ M Beach Club

Plenary Talks

Interfacial Design and Engineering for High Performance Aqueous Zinc Ion Batteries

Zaiping Guo*

School of Chemical Engineering and Advanced materials, The University of Adelaide, SA 5005, Australia

Abstract:

Rechargeable aqueous zinc-ion batteries (RAZBs) have been revived as complementary to LIBs as a result of the intrinsic safety of aqueous electrolytes and the attractive properties of Zn metal anode, including high theoretical capacity (820 mA h g^{-1} and $5855 \text{ mA h cm}^{-3}$), low redox potential, and abundant resources. Despite these unique advantages, their practical application is largely impeded by their inferior cycling stability and their low Zn plating/stripping Coulombic efficiency (CE). Zn metal is thermodynamically unstable in conventional aqueous electrolytes, and consequently, side reactions (e.g., H_2 evolution and Zn corrosion) occur at the electrode-electrolyte interface. In addition, the initial Zn nucleation is normally localized during the process of Zn deposition, leading to an uneven interfacial electric field and tip-effect-derived dendrite formation. These notorious issues of dendrite growth and side reactions are even more critical under practical conditions such as high plating/stripping current density, lean electrolyte, and limited excess Zn. In this talk, I will present some of our recent work in addressing these issues of the Zn anodes via electrolyte optimization and interfacial engineering.

Biography:

Professor Zaiping Guo is an Australian Laureate Fellow at School of Chemical Engineering, The University of Adelaide. She received her PhD from University of Wollongong in 2003 and was elected to Fellow of the Australian Academy of Science 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, and 2022. She was also awarded 2020 NSW Premier's Prizes for

Molecular Aggregates -- Functional Mesoporous Materials Assembled by Single Micelles

Dongyuan Zhao*

Department of Chemistry, Laboratory of Advanced Materials and Collaborative Innovation Center of Chemistry for Energy Materials, Fudan University, Shanghai 200433, P. R. China

Abstract:

Functional mesoporous materials are a class of porous solids with a pore size of 2-50 nm. They not only possess unique properties such as a high specific surface area, large pore size and uniform and controllable pore volume, but also have excellent optical, electrical and magnetic properties of inorganic functional nanoparticles. In this lecture, we mainly demonstrate the recent progress in the orientation assembly controllable synthesis of multilevel structural functional mesoporous materials through interface molecular aggregation control. Based on the idea of interface assembly regulation, we have developed a series of new methods for the synthesis of multilevel structural functional mesoporous materials such as single micelles. Here we mainly introduce a method for superassembly using single micelles as a structural unit. Using this approach, we can controllably prepare a series of novel multilevel structural functional mesoporous materials, which not only have unique and uniform morphology, but also have controllable mesoscopic pore structure, high specific surface area, large pore volume and open pore. At the same time, we will also introduce the recent applications of functional mesoporous materials in catalysts, electrode materials, thermal insulation materials, dielectric materials and other fields.

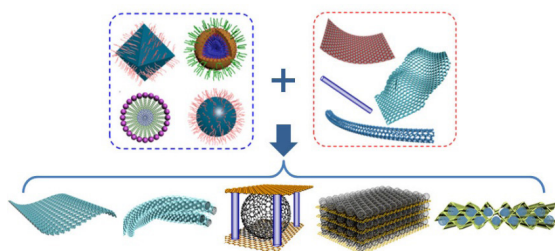


Figure 1. Modular super-assembly of hierarchical superstructures from monomicelle building blocks

Biography:

Professor Dongyuan Zhao, Dean of School of Chemistry and Materials at Fudan University, Senior Editor for ACS Central Science. He has devoted himself for more than 25 years to the interfacial assembly and synthesis of ordered functional mesoporous materials for the applications in energy, environment, and biology. Prof. Zhao received many awards including: National Natural Science Award (1st Grade, 2020); IMMA Achievement Award, 2008; The Ho-Leung-Ho-Lee Award, 2009; TWAS-Lenovo Science Prize, 2016; Khwarizmi International Award, 2019; JCIS Darsh Wasan Award, 2018; Chemistry Contribution Award, China Chemical Society, 2018; ACS Nano Award, 2021 and achieved a series of innovative research results in *Science*, *Nature*, and *Nat. Chem*, *Nat. Mater.*, *Sci. Adv.*, *J. Am. Chem. Soc.*, and other top journals have published over 850 papers which have been cited more than 140,000 times.

Carbon-Based Materials for Catalytic Energy Conversion and Environmental Remediation

Shaobin Wang*

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Abstract:

Nowadays, energy crisis and environmental pollution are the important issues in the world. Catalytic reaction using solar light is 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. Photocatalytic water splitting has been suggested as an approach for solar energy conversion and hydrogen production. Graphitic carbon nitride (CN) has been widely tested as a metal-free photocatalyst for various applications in solar energy conversion and environmental remediation.

In the past years, we have prepared different CN-based materials for photocatalytic water splitting to hydrogen and oxygen, ammonia decomposition and water pollutant degradation. We tested heterojunctions for hydrogen generation and Co-loaded CN for oxygen generation. In general, those materials have demonstrated effective performance in water splitting. In addition, van der Waals (VDW) heterojunctions in a 2D/2D contacts significantly improve the photocatalytic performance. Moreover, CN-supported single-atom transition metals can also demonstrate solar light-driven photocatalytic gaseous NH_3 splitting and pollutant degradation.

Biography:

Prof. Shaobin Wang obtained a PhD from the University of Queensland. He has been a John Curtin Distinguished Professor at Curtin University and is now a Laureate Professor at the University of Adelaide. His research interests focus on nanomaterial synthesis and application for adsorption and catalysis, fuel and energy conversion and environmental remediation. He was 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 and Energy as well as an editorial board member of several international journals.

Phase Engineering of Nanomaterials (PEN)

Hua Zhang*

*Department of Chemistry, Hong Kong Branch of National Precious Metals Material Engineering Research Center (NPMM), City University of Hong Kong, Hong Kong, China
Shenzhen Research Institute, City University of Hong Kong, Shenzhen, 518057, China*

Abstract:

In this talk, I will summarize the recent research on phase engineering of nanomaterials (PEN) in my group, particularly focusing on the rational design and synthesis of novel nanomaterials with unconventional phases for various promising applications. For example, by using wet-chemical methods, for the first time, we have successfully prepared novel Au nanostructures (e.g., the hexagonal-close packed (*hcp*) 2H-Au nanosheets, 4H-Au nanoribbons, and crystal-phase heterostructured 4H/*fcc* and *fcc*/2H/*fcc* heterophase Au nanorods), epitaxially grown

metal nanostructures on the aforementioned unconventional Au nanostructures and 2H-Pd nanoparticles, and amorphous/crystalline heterophase Pd, PdCu, Rh and Rh alloy nanosheets. In addition, by using gas-solid reactions, metastable 1T'-phase group VI transition metal dichalcogenides (TMDs), e.g., WS₂, WSe₂, MoS₂, MoSe₂, WS_{2-x}Se_{2(1-x)} and MoS_{2-x}Se_{2(1-x)}, have been prepared. Moreover, the salt-assisted 2H-to-1T' phase transformation of TMDs have been achieved, and the phase transformation of TMDs during our developed electrochemical Li-intercalation process has been observed. Impressively, the lithiation-induced amorphization of Pd₃P₂S₈ has been achieved. Currently, my group focuses on the investigation of phase-dependent physicochemical properties and applications in catalysis, (opto-)electronic devices, clean energy, chemical and biosensors, surface enhanced Raman scattering, photothermal therapy, etc., which we believe is quite unique and very important not only in fundamental studies, but also in future practical applications. Importantly, the concepts of phase engineering of nanomaterials (PEN), crystal-phase heterostructures, and heterophase nanomaterials are proposed.

Biography:

Hua Zhang is the Herman Hu Chair Professor of Nanomaterials at City University of Hong Kong. He completed his Ph.D. at Peking University (1998). As a postdoctoral fellow, he joined Katholieke Universiteit Leuven (1999) and moved to Northwestern University (2001). After working at NanoInk Inc. (USA) and Institute of Bioengineering and Nanotechnology (Singapore), he joined Nanyang Technological University in 2006 and moved to City University of Hong Kong in 2019. His current research focuses on phase engineering of nanomaterials (PEN), especially the preparation of novel metallic and 2D nanomaterials with unconventional phases, and epitaxial growth of heterostructures for various applications.

From Intelligent Nano Materials to Hydrovoltaic Systems

Wanlin Guo*

Key Lab. of Intelligent Nano Materials and Devices of MoE, State Key Lab. of Mechanics and Control of Mechanical Structures, Institute for Frontier Science of Nanjing University of Aeronautics and Astronautics, 29, Yudao Street, Nanjing, 210016, China.

Abstract:

Our understanding of the nature and universal and our ability of creation and production depend on how small we can see (spatial scale), how fast we can capture (temporal scale) and how weak signal we can distinguish (energy scale). When the spatial scale goes down from macroscale to micro-, nano- and pico-meter scale, temporal scale reduces from second to femto- to atto-second, and more importantly, the related energy scale of an externally applied field drops for eighteen orders from joule to atto-joule (1 nN times 1 nm = 6.42 eV), falling into the energy scale of the local fields of matter which consist of electronic structures, charge, molecular orbital and spin states, or well enter the regime of quantum mechanics. Therefore, at nanoscale, matters show distinctly different performances from their bulk materials mainly due to the strong coupling between the local fields of matter and external applied fields, turning common materials such as carbon, even insulators, into functional nanomaterials with exceptional properties we expected for nanoelectronics, spintronics as well as energy conversion devices. Physical mechanics, a combination of classical mechanics with quantum mechanics to understand the structure-function correlation of matters, has witnessed its golden age in recent decades. Now with nanotechnology entering its fourth decade and nanoscience transforming into picoscience, our ability in spatial, temporal and

energy resolutions has experienced revolutionized advance. This revolution opens up a new way for new functional devices and efficient energy conversion technology.

Just as water breeds life, when water meets nanomaterials, the local fields of water molecules, ions, protons and nanomaterials will inevitably be coupled at air-liquid-solid interfaces, harvesting electricity from water by the novel hydrovoltaic effects, creating new generation artificial intelligence, leading to intelligent hydrovoltaics for understanding our brain. generating new intelligent characteristics and green energy technology.

In this talking, 1) the rich force-electric-magnetic-optic-thermal coupling functional characteristics and the latest progress of nanomaterials will be reviewed; 2) the multi-field coupling effect at the solid-liquid interface of nanomaterials and water, especially the hydrovoltaic effects, and the recent advances; 3) consider the sustainable development challenge, the basic scientific questions of hydrovoltaic energy, ecology, and intelligence will finally be discussed.

Biography:

Dr. Wanlin Guo, Academician of Chinese Academy of Sciences, founder and director of the Key Laboratory of Intelligent Nano Materials and Devices of Ministry of Education and the Institute for Frontier Science of Nanjing University of Aeronautics and Astronautics. His current research focuses on intelligent nano materials and devices, novel conception and technology for efficient energy conversion, molecular physical mechanics for neuronal signaling and molecular biomimics, as well as strength and safety of aircraft and engine. He has published more than 400 peer-reviewed journal papers on *Nature* series, *Phys. Rev. Lett.*, *J. Am. Chem. Soc.*, *Adv. Mater.*, *J. Mech. Phys. Solids*, *Nano Lett.*, etc. He received the National Science Foundation of China for Distinguished Young Scholars in 1996 and the position of Cheung Kong Scholars in 1999. He obtained the National Nature Science Prize of China in 2012 for his contribution to physics mechanics, the ICCES Eric Reissner Award in 2019 for his sustained contributions to the integrity and durability of aerospace structures, and to nano-mechanics, and the Ho Leung Ho Lee Award for Technological Progress.

Endowing Nonprecious Materials with Catalytic Capability for Green and Sustainable Production of Chemicals and Fuels

Huijun Zhao*

Centre for Catalysis and Clean Energy, Griffith University, Queensland, 4222, Australia

Abstract:

Catalysts play an essential role for over 90% of current chemicals manufacturing processes and hold a central key for clean energy and green chemicals manufacturing future. For production of fuels and chemicals, the majority of high-performance catalysts currently in use are made of precious metals-based materials, however, unsustainable due to their expensive and scarcity nature. The development of cheap and plentiful materials-based catalysts is therefore vital for economical viable future of chemicals manufacturing industry. Unfortunately, the most of nonprecious materials in their pristine forms possess poor catalytic activity. As such, exploring effective means to endow nonprecious materials with superior catalytic capability is a must, but highly challenging.

It is well known that to date, the petroleum-based feedstocks are almost exclusively used for industrial production of chemicals and fuels, which emits CO₂ that is environmentally damaging and is unsustainable due to the rapid depletion of petroleum resources. Therefore,

an ability to use cheap and earth-abundant biomass and simple molecules such as N_2 , CO_2 , O_2 , H_2O and $NaCl$ as feedstocks to produce chemicals and fuels would reduce not only CO_2 emission, but also our reliance on petroleum resources.

This presentation intends to illustrate the pressing issues of developing real-world applicable catalysts and effective approaches to activate nonprecious materials as high performance catalysts for catalytic conversion of biomass and simple molecules into valuable chemicals and fuels. A number of findings resulting from our recent investigations will be used to exemplify the effectiveness and applicability of new synthetic approaches and activation principles that empower the nonprecious materials with superior catalytic capabilities toward a spectrum of important thermo- and electro-catalysis reactions for green production of fine and commodity chemicals.

Biography:

Professor 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 Australian Academy of Technological Sciences & Engineering (FTSE), the Fellow of Royal Society of Chemistry (FRSC) and the Fellow of the Royal Australian Chemical Institute (FRACI). He has extensive expertise in functional materials, energy conversion and storage, catalysis and sensing technologies. He 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.

Theoretical Design of Two-Dimensional Visible Light-Driven Photocatalysts for Overall Water Splitting

Jinlong Yang*

University of Science and Technology of China, Hefei, Anhui 230026, China; Hefei National Laboratory, Hefei, Anhui 230088, China

Abstract:

Hydrogen production from water via photocatalytic water-splitting has attracted great interest due to the increasing challenge from energy and environment. The light harvest, electron-hole separation and catalytic activity are keys to enhance the efficiency of solar energy utilization, which stimulates the development of high-performance photocatalysts. Two-dimensional (2D) materials have attracted much attention due to their extremely large specific surface area, shortened carrier migration path and excellent optical properties, but it is still a challenge to realize overall water splitting under visible light with 2D materials photocatalysts experimentally. Density functional theory (DFT) based first-principles calculations provides a quicker and lower cost approach in materials design than experimental exploration. In this report, recent advances in design of 2D materials photocatalysts, including chemical decoration, molecular engineering, building heterostructures, perpendicular electric field introduction and machine learning are systematically presented from a theoretical perspective. Future opportunities and challenges in theoretical design of 2D materials photocatalysts toward overall water splitting are also included.

Biography:

Jinlong Yang is an academician of the Chinese Academy of Sciences, a professor and vice president of the University of Science and Technology China (USTC). He received his PhD

degree in condensed matter physics from USTC in 1991. He was the recipient of the Young Chemist award from the Chinese Chemical Society and the Second Class Prize of National Natural Science, and was selected as American Physical Society fellows for 2011. His research interests focus on the development of the first principles methods and their applications to clusters, nanostructures, solid materials, surfaces, and interfaces.

A New Electrolysis Technology for Hydrogen Generation

Zongping Shao^{1*} Jlayi Tang*

¹WASM: Minerals, Energy & Chemical Engineering, Curtin University, Kent Street, Bentley, WA 6845, Australia

Abstract:

Cost-effective and scalable green hydrogen production from water electrolysis is crucial to achieve a net-zero emission future. Progress on water electrolysis technologies has long been made towards materials design and device assembly optimization to improve cost effectiveness. However, expensive iridium-based electrocatalyst, pure water feedstock, low current density, and energy efficiency limit state-of-the-art water electrolysis, i.e., alkaline and polymer exchange membrane water electrolyzers based on liquid-water feeding for large-scale implementation. Here we propose a revolutionary semi-vapor electrolysis (SVE) system for cost-effective hydrogen generation that adopts low temperature vapor electrolysis at anode while keeps water liquid circulation at cathode. The SVE process requires no additional energy input as compared to conventional water liquid electrolysis while enabling the direct use of a wide range of water resources without pre-treatment. In addition, much cheaper and intrinsically more active ruthenium oxide can be used under the circumstances of SVE to avoid dissolution, which achieves an ultrahigh current density of 4.67 A cm⁻² at 1.8 V and superior stability under practical 1 A cm⁻² for hydrogen production. Techno-economic assessment suggests significant hydrogen cost reduction due to the improved energy efficiency, reduced material cost and simplified system, and by-product profits, demonstrating the scalability of the as-proposed SVE.

Biography:

Zongping Shao is a John Curtin Distinguished Professor at Curtin University. His major research areas are located at (photo)electrochemical energy storage and conversion and new energy materials. Up to now, Prof. Shao has published about 800 materials-related papers in various reputed journals, like Nature (5), Science (1), Nature Energy (2) Nature Catalysis (1), Nature Communications (13), and Science Advances (1) He is also selected as world-highly cited researcher by (Thomson Reuters) Clarivate Analytics for the years, 2014, 2017-2023, in particular, he is highly cited in two fields of Materials Science and Chemistry at 2022 and 2023.

Session: Materials Science and Engineering

Keynote Talks

Novel Materials Chemistry for Applications in Energy Storage and Conversion

Nicola Pinna*

Department of Chemistry, Humboldt University of Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany

Abstract:

The current trend in various energy applications, ranging from batteries to electrolyzers, lays in the control of structural, physicochemical and morphological properties of materials and their interfaces. During this presentation, recent scalable strategies for nanostructured materials synthesis, targeting energy and environmental applications will be discussed. Especially, we will focus on one-pot strategies for the fabrication of hybrid and complex nanomaterials focusing on the importance of the organic inorganic and inorganic-inorganic interfaces. Among the examples presented, we will discuss the synthesis of complex nanostructures and the stabilization of metastable phases for applications in energy, catalysis and environmental remediation. We will see that nowadays the available strategies allow a control in terms of composition, crystalline structure, morphology and nanostructuring that would have been unimaginable just few years ago. Finally, the open challenges the field is currently facing and possible further developments which are needed to meet the always growing demand for high performing materials will be also discussed.

Biography:

Nicola Pinna received his Ph.D. in physical chemistry from the Université Pierre et Marie Curie (Paris) in 2001. He has since worked at the Fritz Haber Institute of the Max Planck Society (Berlin), the Max Planck Institute of Colloids and Interfaces (Potsdam), the Martin Luther University of Halle-Wittenberg, the University of Aveiro (Portugal), and the Seoul National University (Korea). In July 2012 he joined the Department of Chemistry of the Humboldt University of Berlin as professor of inorganic chemistry. From July 2016 to April 2021, he was also head of the Department. His research activity focuses on the development of novel materials chemistry routes to nanostructured materials for energy and environmental applications.

Mitigating Challenges of Aqueous Zn batteries

Hong Jin Fan*

Nanyang Technological Universities, Singapore

Abstract:

Rechargeable Zn aqueous batteries (ZAB) are being widely and extensively studied. Despite the tremendous progress in fundamental understanding and battery performance by rational design of electrode materials, electrolytes and device architectures, mitigating the known formidable challenges of ZAB is still the holy grail. The challenges include electrode material instability, low working voltage and energy density, and complicated reactions. Our group has been actively working various aspects of ZAB from electrode materials design, anode protection, electrolyte engineering, to new battery couples. In this talk I will present some of our strategies for Zn anode stabilization, durable zinc-iodine and zinc-sulfur aqueous batteries.

Biography:

Dr Fan received PhD from National University of Singapore in 2003. After his postdoc research at Max-Planck-Institute, Germany and the University of Cambridge, he joined Nanyang Technological University in 2008. Dr Fan has been working on energy materials and devices, including electrocatalysis for hydrogen generation and new-generation batteries. He has co-authored 300 journal papers with an H-index of 100 (WoS) and has been recognized as *Highly Cited Researcher* since 2016. He is currently the Editor-in-Chief of *Materials Today Energy* (2022 IF: 9.3), and editorial/advisory board member of journals including *Energy and Environmental Sciences*, *Small*, *Advanced Science*, *eScience*, *Next Energy*, etc.

Two-Dimensional Materials for Next-Generation Electronics and Optoelectronics Technologies

Sumeet Walia*

RMIT University, School of Engineering, Melbourne, Australia 3001

Abstract:

Atomically-thin materials possess unique intrinsic properties and are amenable to a range of tuning techniques. We harness these properties underpinned by application demand and work with industry to translate into end-user products.

Firstly, we synthesise a variety of atomically-thin metal oxides, mono/dichalcogenides and elemental 2D materials using solid, liquid and vapour phase techniques guided by application.

Our fundamental advances have been uncovering the origins of oxidative degradation in few-layer black phosphorus (BP) and subsequently proposing an ionic liquid-based approach to prevent ambient degradation of BP. Using defect engineering, we have demonstrated neuromorphic vision and processing sensors. We have explored the use of hybrids of dissimilar materials to enhance electronic and optical performance. Ultra-thin layers have been used to develop one of the world's thinnest photodetectors that can sense all shades of light from UV-infrared. We further study strain-tunability in low-dimensional structures via integrating them onto elastomeric platforms.

Using a cross-disciplinary approach, we deploy multifunctionality of these new material systems into solving technological challenges for industry partners across sectors that require novel materials and functions to be integrated into their products.

Biography:

Sumeet is a Professor of Materials and electronics engineering at RMIT University in Melbourne. He leads a research group that focuses on discovering and manipulating fundamental properties of materials for applications across energy, nano/optoelectronics, sensors and healthcare.

He has co-authored over 140 peer reviewed publications including authoritative reviews in prestigious journals, a named inventor on eleven patents and editor of two books for the CRC Press.

His scientific and leadership contributions have been recognised through several national and international awards including the Eureka Prize for Science leadership and the MIT Technology Review's Top 10 Innovators in APAC.

Recent Alloy Design and Process Development for 3D Printed Aerospace Applications in Monash Centre for Additive Manufacturing

Aijun Huang*

Monash University, Australia

Abstract:

Additive manufacturing (AM) is a revolutionary technology which offers mass potential for aerospace metallic parts. Although many additive manufactured aerospace parts are in service in last a few years, the overall implementation of AMed parts is still insignificant due to intrinsic high cost, unpredictable defects and insufficient mechanical properties. This talk will demonstrate application driven research efforts in Monash Centre for Additive Manufacturing to address above hurdles. Significant improvement in mechanical properties and defects control for AMed aerospace parts was achieved via alloy design, microstructure manipulating and hybrid manufacturing process development. A perspective of Australian metal additive manufacturing industry will also be discussed.

Biography:

Professor Aijun Huang holds a PhD from the University of Birmingham, UK. He is a Fellow, Chartered Engineer and Chartered Scientist of the Institute of Materials, Minerals and Mining UK. He is currently the Director of Monash Centre for Additive Manufacturing and a full professor in the Department of Materials Science and Engineering, Monash University

Prior to his appointment at Monash University, Prof. Huang was an industry technical expert for a number of multinational corporations. Prof Huang held the position of the Executive Vice President of the High-Performance Materials Business Unit which exclusively manufacturing all aerospace metallic materials in Baosteel Group; a Fortune Global 500 company. From 2006 to 2012, Prof Huang was the Titanium Specialist of Rolls Royce Derby globally leading the titanium and titanium aluminides fundamental research within the company where he was elected to the Rolls Royce Engineering Leadership List in 2011

Professor Aijun Huang's research covers the entire spectrum of metal additive manufacturing (AM). Research efforts have covered; AM specific alloy design; metal powder manufacturing technology; component design for AM; AM process optimisation; post-AM process development including inspection, qualification, and certification of final AM parts. Conventional physical metallurgy of aerospace materials particularly titanium and Ni-based superalloy has also part of his research portfolio.

Harnessing Renewables for Smart Materials: Research to Commercialization

Mohini Sain^{*1}, Omri Menashe¹, Viktoriya Pakerenko¹

¹Department of Mechanical and Industrial Engineering, University of Toronto, Canada

Abstract:

Biomass is an important natural source of global climate solution. Over past 20 years Biomass became a centre point for talks around the world. Although there has been significant progress to develop biomass plantation and biomass oil production with sustainable management techniques and policy, it is important to note that global perception of industry needs more disruptive technologies and policy framework to bring Biomass industry in the mainstream material and energy sector.

In Asia and Middle East Biomass plantation has been growing by more than 10% over past 20 years. When primary driver for growth is biomass oil for food and industrial usage, biomass generated from biomass oil became a significant resource for secondary use sectors including first generation ethanol from biomass leaf and other biomass biomass and more recently biomass leaf are finding more applications in packaging and advanced materials including molded nanobiocomposites for speciality application.

This paper will present two aspects of potential mass utilization of biomass leaf and biomass for packaging materials and energy applications. By demonstrating unique manufacturing technology for fast and precision molding as well as isolation and drainage technology to sustainably manufacture nanofibrillated biomass cellulose from sugar biomass fibres produced by a chemo-mechanical approach, thus opening a new way to utilize waste products more efficiently. Chemical pre-treatments, namely delignification and mercerization processes, were initially involved to extract the sugar biomass cellulose. Then, mechanical pre-treatment was performed by passing the sugar biomass cellulose through a refiner to avoid clogging in the subsequent process of high pressurized homogenization. The fibre and biomass leaf direct utilization engineering science developed at UofToronto promises to be a very versatile material by having a huge potential in many applications, encompassing bio-packaging to scaffolds for tissue regeneration.

Biomass biomass-based biorefineries have emerged as an effective and productive pathway to secure bioproducts and green energy in future. Biomass biomass lignin, an abundantly available biomass sourced from pulp industry's waste stream, provides various opportunities in the development of value-added bioproducts and green fuels. However, due to the high level of color and low biodegradability, lignin is categorized as a serious pollutant particularly in the aquatic ecosystem. This present will provide a more holistic approach towards Biomass biomass and biomass leaf utilization and their potential commercial opportunities in a broad range of value chains including biomedical, packaging, transportation and electronics.

ROOM A**Session: Materials for Energy Conversion and Storage****Keynote Talks****Electrochemical Engineering and Direct Ink Writing 3D Printing: Cost-Effective Production of 2D Nanomaterials and their Bespoke Assemblies****Yu Lin Zhong****School of Environment and Science, Queensland Micro- and Nanotechnology Centre, Griffith University, Australia***Abstract:**

Electrochemical engineering is a powerful technique that has been applied on industrial scale to cost-effectively produce valuable chemicals and materials that are otherwise difficult to produce via traditional chemical synthesis (i.e. utilising heat or catalysts). As such, it is a highly viable method to overcome the bottleneck in the commercialisation of novel 2D nanomaterials (production cost) and enabling them, through in situ modifications, for their niche application in flexible and energy-related devices. We have employed a combination of highly robust boron-doped diamond (BDD) with a wide electrochemical potential window and commercially available fused deposition modelling (FDM) 3D printing to fabricate a scalable packed-bed electrochemical reactor (PBER) for GO production. In our recent work, the niche feature of two-dimensional carbides and nitrides of transition metals (MXenes) was capitalised in our packed-bed electrochemical reactor to produce MXenes at an unprecedented reaction rate and yield with minimal chemical waste. A simple NH_4F solution was employed as the green electrolyte, which could be used repeatedly without any loss in its efficacy.

Regarding bespoke assembly, we have demonstrated a new effective formulation for 3D printing of conductive PDMS/graphene ink by using an emulsion method to form a uniform dispersion of PDMS nanobeads, EGO and PDMS precursor binder. Due to the unique hybrid structure of PDMS and EGO sheet, the 3D printed EGO/PDMS nanocomposite possesses high, linear and reproducible sensitivity that is suitable for application as skin-attachable wearable health monitoring device. To power the wearable devices, we have introduced a highly printable MXene ink that was prepared by incorporating a surfactant (C12E9) into the MXene hydrogel. The formulated nanocomposite ink facilitates the alignment of the MXene flakes during extrusion as well as the formation of the aligned micro- and sub-microsized porous structures, leading to the improved electrochemical performance of the printed microsupercapacitor.

Biography:

A/Prof Yulin Zhong completed his PhD in Chemistry at the National University of Singapore (NUS) and did his post-doctoral training at Princeton University (2009) and Massachusetts Institute of Technology (2011). After spending three years in the USA, he worked as a Research Scientist at the Institute of Bioengineering and Nanotechnology, A*STAR Singapore, (2012) and thereafter, as an ARC DECRA Fellow at Monash University (2013). In 2016, he accepted a

Senior Lecturer position at Griffith University, was promoted to Associate Professor in 2020 and awarded the ARC Future Fellowship in the same year. Currently, he serves as the Treasurer in the Electrochemistry Division of the Royal Australian Chemical Institute.

Atom-Scale Defect Manipulating of 2D Materials for Boosted Electrocatalytic Properties

Junjie Guo^{1*}, Haixia Zhang¹, Yanhui Song¹, Peizhi Liu¹

¹Key Laboratory of Interface Science and Engineering in Advanced Materials of Ministry of Education, Taiyuan University of Technology, Taiyuan 030024, P.R.China

Abstract:

The evolution of pivotal renewable energy technologies covering fuel cells and electrocatalytic water splitting hold great potential to alleviate the energy crisis and reduce environmental pollution. These promising alternative technologies, however, are limited by the sluggish reaction kinetics and high-cost catalysts. Precisely manipulating the microstructure and local coordination environment of two-dimensional (2D) metal-based catalysts is an effective way to enhance their intrinsic catalytic activity, facilitate charge/mass transport, and thus boost the electrocatalytic performance for hydrogen evolution reaction (HER), oxygen reduction reaction (ORR), and oxygen evolution reaction (OER).

In this study, the atomic configurations of atomically-thin 2D electrocatalysts, such as metal atom doped graphene, metal nanosheets, and metal (hydr)oxide nanosheets, were analyzed by using STEM to study the atomic origin of their improved electrochemical properties. It is found that the atomic defects in these 2D materials, such as nanopore, heteroatom dopant, and localized amorphous region, etc., play the key role to boost their electrocatalytic properties.

Biography:

Dr. Junjie Guo is a professor of Taiyuan University of Technology. He received PhD. in materials science from Tohoku University, Japan in 2010. He was engaged in postdoctoral research at Oak Ridge National Laboratory, United States from 2011-2014.

His current research focuses on the atomic-scale structure manipulating and characterization of two dimensional (2D) materials for improved electrochemical properties. So far, he has published more than 150 papers, including Nature Communications, Advanced Science, Nano Energy, Acta Materialia, Small.

Ceramic Materials for Energy Conversion: From Joining and Integration Challenges to Recycling Strategies

Federico Smeacetto*

Department of Applied Science and Technology, Politecnico di Torino, Italy

Abstract:

Hydrogen-related technologies are essential to enable deep decarbonization of the energy system. Advanced glass and ceramic materials play a key role in enhanced efficiency and durable electrochemical energy conversion systems, such as reversible solid oxide cells,

electrolyzers, and proton conducting membranes. Current solutions and challenges related to the design, processing, microstructure-property-performance relations of different glass and ceramic-based systems and their integration process, specifically developed in the field of hydrogen-related technologies are presented. The presentation highlights how advanced glass and ceramic-based materials offer huge potential for disruptive innovations in the fields of energy conversion and storage, pointing out some unanswered questions about their durability, reliability, challenges, and perspectives for further research. However, since the demand for green hydrogen production is going to increase, the request for electrolyzers and the materials required for their production will also increase dramatically, thus highlighting the importance of recovery and recycling. Potential strategies for recycling routes of high-temperature ceramic components including critical raw materials, through hydrothermal treatment from batch to continuous processing in a pilot plant, are also reviewed and discussed.

Biography:

Federico Smeacetto, Ph.D., *Full Professor of Materials Science and Technology* at Politecnico di Torino, Italy. His research interests currently deal with required engineering solutions for designing, processing and characterizing functional glass and ceramics as joining and coating materials for energy conversion. Post-doc researcher at Imperial College, London UK, and University of Hertfordshire, UK. He is supervising a research group of 6+ post-doc researchers and PhDs; a member of the Board of the Ph.D. School of Materials Science and Technology at the Politecnico di Torino. Principal investigator of EU-funded projects and contracts mainly related to hydrogen technologies; recently awarded the prestigious *Acers Global Ambassador from The American Ceramic Society*.

Efficient Solution to Suppress Charge Recombination derived from Bad P-Sn interaction

Ji-Hyun Jang*

Ulsan National Institute of Science and Technology, Republic of Korea

Abstract:

Hematite (Fe_2O_3) has been widely used as a photoanode in photoelectrochemical water splitting (PEC) for green hydrogen production. Although doping has proven effective in enhancing the solar-to-hydrogen (STH) conversion efficiency of hematite by addressing its poor transport behavior, in this study, we reveal that unintentional Sn doping causes severe charge recombination in the P-doped hematite system. We discovered that the strong electrical repulsion created by excess electrons from n-type P^{5+} and Sn^{4+} dopants induces the structural destabilization in the hematite lattice, resulting its poor PEC performance. By obtaining the structural stability via titanium (Ti) doping, $\text{P}:\text{Sn}:\text{Ti}-\text{Fe}_2\text{O}_3$ showed improved PEC performance (3.44 mA cm^{-2} at $1.23 \text{ V}_{\text{RHE}}$), about 680% higher than that of $\text{P}:\text{Sn}-\text{Fe}_2\text{O}_3$. With the deposition of a cocatalyst, the photocurrent density of $\text{NiFeO}_x/\text{P}:\text{Sn}:\text{Ti}-\text{Fe}_2\text{O}_3$ was 4.30 mA cm^{-2} at $1.23 \text{ V}_{\text{RHE}}$ with a cathodic shift (130 mV) of the onset potential, marking the highest values among P doped Fe_2O_3 studies.

Biography:

Ji-Hyun Jang has been a professor of the school of Energy and Chemical Engineering at UNIST Since 2009 in Korea. She received Ph.D. degree in chemistry from KAIST, Korea, in 2004. From 2004 to 2009, she was with Ned Thomas at Materials Science and Engineering, MIT

as a postdoctoral associate. Her research has been focusing on energy materials including photocatalysis for hydrogen generation and electrocatalysts for energy-storage devices. She is also involved in synthesizing and developing physicochemical properties of the 2D materials. She is currently an Associate Editor of Materials Today Energy.

Hydrogen Evolution *via* Interface Engineered Nanocatalysis

Wei Chen^{1,2*}

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²Department of Chemistry, National University of Singapore, 117543, Singapore

Abstract:

Hydrogen has emerged as a green and sustainable fuel to meet the demand for future global energy. Nowadays the majority of hydrogen is still produced from steam-reformed methane, which is derived from limited fossil resources and greatly increases CO₂ emission. Electrocatalytic hydrogen evolution reaction (HER) enabled by renewable electricity holds great promise as a safe, scalable, low-cost, and environmental-friendly pathway for hydrogen production. To date, noble metals (e.g., Pt, Pd, and Rh) are regarded as the most efficient materials to catalyze the conversion of H₃O⁺ (acid) and H₂O (alkaline) to H₂. In order to maximize the utilization efficiency of noble metals, the rational design and controllable synthesis of catalysts based on the deep understanding of reaction mechanism and structure–activity relationship is crucial for cost-efficient HER catalytic process.

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

Strategies to Boost Electrochemical Reversibility and Performance for Atmospheric Energy Storages

Won-Hee Ryu*

Department of Chemical and Biological Engineering, Sookmyung Women's University, Seoul, Republic of Korea

Abstract:

The escalating demand for advanced energy storage systems to enhance the performance of various electronic devices and equipment is driving innovation in battery energy density. Traditional Li-ion batteries (LIBs), limited by their use of heavy transition metal oxides in cathodes, fall short in achieving theoretical maximum energy density. Additionally, the environmental degradation caused by the mining of these metal minerals necessitates the development of transition metal-free cathode materials.

Air-breathing batteries such as Li-O₂ and Li-CO₂ as atmospheric energy storages have been intensively studied for breakthrough in energy storages due to their remarkable energy density potential. The intrinsic challenges arising from insulating product formation have

been mitigated by developing various types of efficient catalysts. Although efforts have been input to seek suitable catalyst alternatives including solid-phase and soluble-phase, we should further understand O_2 or CO_2 electrochemistry facilitated by the catalysts on the electrode or in the electrolyte. In this presentation, I would introduce several ways to develop catalyst materials and systems for outperforming efficient and sustainable air-breathing cells (Li- O_2 and Li- CO_2 batteries).

Biography:

Prof. Won-Hee Ryu received his M.S. (2007) and Ph.D. (2012) from the Department of Materials Science and Engineering at Korea Advanced Institute of Science and Technology, Korea. He did postdoctoral studies at Yale University (2013–2016). He is currently working as an associate professor of the Department of Chemical and Biological Engineering at Sookmyung Women's University. His research studies focus on the development of functional materials and systems for electrochemical energy storage and conversion. He has been recognized with fellowship and awards including The NatureNet Science Fellows (2014-2016), The Korean Electrochemical Society (KECS) Park Sumun Award (2022), Journal of Materials Chemistry A Emerging Investigators (2022), Journal of Energy Chemistry Young Editorial Board Member (2023-2024), and Sustainable Materials and Technologies Associate Editor (2023-present).

Precise Construction of Porous Carbon Materials for Energy Conversion

Jian Liu^{1,2,3*}

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²*State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

³*DICP-Surrey Joint Centre for Future Materials, Department of Chemical and Process Engineering, University of Surrey Guildford, Surrey, UK*

Abstract:

Rational design and synthesis of porous carbon materials with unique physical-chemical properties (such as versatile micro/nanostructures, abundant pores, and large specific surface area) have gained huge attention because of their promising applications in energy conversion. All these properties and suitability of porous carbon materials used for energy conversion applications are highly dependent on their synthesis strategy. Herein, the purpose of our research is to precisely construct porous carbon materials and to investigate their energy conversion applications, particularly for the conversion of small molecules ($H_2O/N_2/CO_2$) and organic molecules (e.g., cinnamaldehyde/nitrobenzene/phenylacetylene) in electrocatalytic and photocatalytic reactions. For the controllable synthesis of porous carbon, we have proposed two novel strategies: bottom-up self-assembly strategy and top-down "chemical scissoring" strategy. Based on these synthetic methods, carbon materials with various mesostructures, morphologies, and tunable pore size can be successfully achieved. Meanwhile, the utilization of these obtained carbon in varied energy conversion applications are deeply investigated. For example, porous B,N@C electrocatalysts and bowl-shaped carbon nanoreactor with controllable diffusion process can be successfully constructed and showed high performance electrochemical H_2O_2 production. Therefore, the advanced properties and marked advantages of designing and constructing porous carbon are many fold, and show great aid and potential in energy conversion and other applications.

Biography:

Jian Liu is currently a chair professor and head of the School of Chemistry and Chemical Engineering, Inner Mongolia University, China. He obtained his Ph.D. degree in physical chemistry from the Dalian Institute of Chemical Physics, Chinese Academy of Science, China, in 2008, to study inorganic material chemistry and catalysis. He was listed among the 2018–2023 Highly Cited Researchers from Clarivate in cross-field. His current research interests are nanoreactor design, sustainable H₂O₂ photo/electrosynthesis, and CO₂ utilization.

HOMO Energy Level Modulation with Fluorinated Poly(aryl)amines for Wide-Bandgap Perovskite Solar Cells

Thomas J. Macdonald*

University College London, Department of Electronic and Electrical Engineering, Roberts Building, Torrington Pl, London WC1E 7JE, United Kingdom

Abstract:

Fluorination stands out as an effective strategy to narrow the energy gap between HTMs, such as Poly(aryl)amines (PTAA), and perovskite materials. We demonstrate the synthesis of six novel fluorinated PTAA derivatives and present innovative methods for introducing trifluoromethyl (CF₃) groups into PTAA structures. Our investigation, incorporating electrochemical and optical spectroscopy analyses, highlights the significant influence of both the position and quantity of fluorine atoms on PTAA's energy levels. Additionally, we demonstrate that fluorine atoms and CF₃ groups impact orbital level structures differently, advancing our understanding of PTAA's role in PSCs. Importantly, we have fabricated wide-bandgap PSCs with fill factors exceeding 80%, short-circuit current densities surpassing 17 mAcm⁻², and power conversion efficiencies exceeding 17%. Notably, this was achieved without implementing surface passivation, underscoring the potential for optimizing high-performance HTMs in PSCs.

Biography:

Thomas J. Macdonald is an Associate Professor in Electronic Engineering within the Department of Electronic and Electrical Engineering at University College London. He is the recipient of a prestigious University Research Fellowship from the Royal Society and is a former 1851 and Ramsay Fellow. He also holds an Honorary Visiting Researcher position in the Department of Chemistry at Imperial College London. He received his PhD in 2016 from the University of South Australia and has a strong interest in renewable energy. His extensive experience includes the synthesis and modification of functional nanomaterials and the fabrication of third-generation photovoltaics.

Toward Energetic Aqueous Battery: Electrochemistry and Device

Dongliang Chao*

Laboratory of Advanced Materials, School of Chemistry and Materials, Fudan University, Shanghai 200433, People's Republic of China

Abstract:

Recent incidents in organic media-based Li-ion batteries (LIBs), such as the Boeing 787 battery fires in 2013, Samsung Note 7 explosions in 2016, and the Tesla Model S combustions in 2019, have caused severe threats to human health and life. This is an alert that safety is a vital prerequisite for next-generation rechargeable batteries for both consumable electronics and electric vehicles. In this content, aqueous batteries (ABs) offer tremendous competitiveness in terms of safe operation, low cost, facile manufacturing and recycling, together with high power density and tolerance against misuse. We have witnessed the prosperity of various types of rechargeable ABs in the market, such as primary Zn-Mn alkaline battery, valve-regulated lead-acid (VRLA), nickel-cadmium (Ni-Cd), and nickel-metal hydride (Ni-MH) batteries. These batteries possess competitiveness in either economical profit, safety, or environmental influence. However, the market share has been continuously shrinking due to the inadequate energy density of ABs compared with the mainstream LIBs. Here, we will summarize the strategies applied in our group toward energetic ABs from a distinct perspective of different battery components. Finally, we render insights properly for future development of high-energy and reliable ABs.

Biography:

Prof. Chao is now working at Fudan University, serving as Executive Director of the Centre for Aqueous Battery. Prof. Chao's main research activity is high-energy aqueous batteries. He is the Associate Editor of the journal *Materials Today Energy* (IF > 9.3). He has published 1 authored book and >100 journal articles with an H-index of 68 and citations over 21,000. His awards include Innovators Under 35 (MIT Technology Review), Rising Star Australia, DECRA Fellow Award (Australian Research Council), and Global Highly Cited Researcher (2020–2023, Clarivate).

Rational Design of Cathode Materials for Proton-Conducting Solid Oxide Fuel Cells

Lei Bi*

School of Resources Environment and Safety Engineering, University of South China, Hengyang 421001, China

Abstract:

The performance of cathodes has been recognized to be important as it governs the overall fuel cell performance of proton-conducting solid oxide fuel cells (H-SOFCs). We present here two strategies to design cathodes for H-SOFCs in comparison with the well-known triple-conduction (oxygen-ion, proton and electron) cathodes have been established for H-SOFCs recently. The first work is the development of $\text{La}_{0.8}\text{Sr}_{0.2}\text{Sc}_{0.5}\text{Fe}_{0.5}\text{O}_{3-\delta}$ (LSSF) cathode for H-SOFCs. The LSSF cathode is demonstrated to show only proton and electron conduction with little oxygen-ion diffusion ability but exhibits high performance in H-SOFCs. In addition, direct evidence of proton-conduction is observed for LSSF, which is technically difficult before. The second work is the use of nanocomposite cathode for H-SOFCs that boost the H-SOFC performance to a record-high level. More importantly, the interface of the nanocomposite cathode is critical in enhancing the performance, which is demonstrated by first-principles calculations at the atomic level, thin-film studies at the nanoscale level and the prototype fuel cell studies.

Biography:

Lei Bi is a full professor at University of South China, leading a research group for proton-conducting solid oxide fuel cells (H-SOFCs). His research interests cover the development and optimization of key materials for H-SOFCs and the new technologies for fuel cell fabrications, using both the first-principles calculation method and experimental approaches. The exploration of new sintering methods for H-SOFC fabrications is another research interest for him. He has co-authored more than 160 papers with a H-index of 59.

Photoelectrocatalytic Properties of Janus Transition Metal Dichalcogenides

Lin Ju*

School of Physics and Electric Engineering, Anyang Normal University, Anyang 455000, China

Abstract:

Janus two dimensional (2D) materials, refer to layered materials with different surfaces. Due to the unique properties induced by spatial symmetry breaking, as well as the important application prospects in energy conversion, this class of materials has attracted strong research interest from researchers. Based on Janus transition metal dichalcogenides (TMDC), our group has conducted systematic and in-depth studies on the physicochemical properties of this class of special structural materials in recent years. Our studies show that by applying suitable modulation (e.g., applying stress, introducing vacancies, metal doping/adsorption), these materials can be equipped with excellent gas-sensitizing and photoelectrocatalytic properties (e.g., water-splitting reaction, CO₂ reduction reaction, NO reduction reaction, etc.), which makes them potentially valuable for applications in the fields of environmental pollution treatment, energy conversion, and so on.

Biography:

Ju Lin, graduated from the School of Physics of Shandong University, majoring in Microelectronics, with a Bachelor's degree of Science in June 2009, and graduated from the School of Physics of Shandong University, majoring in Condensed Matter Physics, with a Doctor's degree of Science in June 2014. January 2021, appointed as a Special Term Professor of the school of Anyang Normal University. As the first author, he has published 24 SCI papers in Nat. Commun., J. Am. Chem. Soc. and J. Mater. Chem. A, and so on. His papers have been cited over 1900 times, and his H-index is 21.

Energy Conversion and Storage over Carbon-Based Materials with High-Density Active Sites

Ji Liang*

Tianjin University, China

Abstract:

A series of carbon-based noble-metal-free catalysts for oxygen reduction reaction (ORR) has been designed and constructed with the purpose of developing highly efficient but low-cost catalysts for fuel cells, metal-air batteries, or hydrogen peroxide production. Their behaviors have been evaluated from both compositional and structural points of view. The principles in designing these advanced carbon materials are also applicable to other critical energy

storage and conversion processes, including electrochemical nitrogen reduction, ammonia oxidation, and metal ion batteries.

Biography:

Prof. Ji Liang received his Ph.D. degree from the University of Adelaide in 2014. After a T. S. Ke Fellowship in the Chinese Academy of Sciences and an ARC DECRA fellowship in the University of Wollongong, he joined the School of Materials Science and Engineering, Tianjin University in 2019. His research interests are in the design of functional carbon-based materials for electrochemical catalysis and energy storage applications. He has published over 140 papers in carbon-based functional materials, which have attracted over 14000 citations. He has an H-index of 47 and is on Stanford's list of World Top 2% scientists. He is an editorial board member of the Journal of Energy Chemistry, Carbon Energy, and EcoMat.

Rational Molecular Design of Carbonyl Compounds for Lithium-Ion Batteries

Yu Jing*

Nanjing Forestry University, Longpan road No.159, Nanjing, China

Abstract:

Lithium-ion batteries (LIBs) are important electrical energy storage devices, but are challenged by high cost and low safety due to the use of inorganic electrode materials. The development of cheap, environmentally friendly and electrochemically active organic electrode materials is essential to promote the sustainable development of LIBs.¹ In view of the problems of easy dissolution in aprotic electrolytes and poor cyclic stability of organic electrode materials, We systematically study the electrochemical activity and stability of carbonyl organic materials as electrode materials for LIBs. By integrating multi-scale theoretical simulations and experiments, we clarify the effects of different molecular skeletons and substitution functional groups on the theoretical capacity, redox potential and molecular polarity of carbonyl molecules,² propose deference in molecular polarity index a simple descriptor to quantify their solubility, reveal the inherent connection between molecular composition and electrochemical activity and solubility, establish effective strategies to regulate the electrochemical activity and solubility of carbonyl organic materials,³ and finally design potential organic electrode materials with high electrochemical activity and high stability. Our investigation will provide reliable guidance for the development of green and sustainable electrode materials.

References:

Xinyue Zhu; Youchao Yang; Xipeng Shu; Tianze Xu; **Yu Jing***. Computational Insights into the Rational Design of Organic Electrode Materials for Metal Ion Batteries, *WIREs Computational Molecular Science*, **2023**, 13: e1660.

Xinyue Zhu; **Yu Jing***. Natural Quinone Molecules as Effective Cathode Materials for Nonaqueous Lithium-Ion Batteries, *Journal of Power Sources*, **2022**, 531: 231291.

Xipeng Shu; Liang Hu; Thomas Heine*; **Yu Jing***. Rational Molecular Design of Redox-Active Carbonyl-Bridged Heterotriangulenes for High-Performance Lithium-Ion Batteries, *Advanced Science*, **2024**, 11: 2306680."

Invited Talks

Manipulating Nb-Doped SrFeO_{3-δ} with Excellent Performance for Proton-Conducting Solid Oxide Fuel Cells

Hailu Dai^{1*}, Hongzhe Du¹, Samir Boulfrad², Shoufu Yu³, Lei Bi³, Qinfang Zhang¹

¹Yancheng Institute of Technology, China

²College of Science & Engineering, Hamad Bin Khalifa University, Qatar

³School of Resource Environment and Safety Engineering, University of South China, China

Abstract:

The Nb-doped SrFeO_{3-δ} material is used as a cathode in proton-conducting solid oxide fuel cells (H-SOFCs). First-principles calculations show that the SrFe_{0.9}Nb_{0.1}O_{3-δ} (SFNO) cathode has a lower energy barrier in the cathode reaction for H-SOFCs than the Nb-free SrFeO_{3-δ} cathode. Subsequent experimental studies show that Nb-doping substantially enhances the performance of the SrFeO_{3-δ} cathode. Then, oxygen vacancies (Vo) were introduced into SFNO using the microwave sintering method, further improving the performance of the SFNO cathode. The mechanism behind the performance improvement owing to Vo was revealed using first-principles calculations, with further optimization of the SFNO cathode achieved by developing a suitable wet chemical synthesis route to prepare nanosized SFNO materials. This method significantly reduces the grain size of SFNO compared with the traditional solid-state reaction method, although the solid-state reaction method is generally used for preparing Nb-containing oxides. As a result of defect engineering and synthesis approaches, the SFNO cathode achieved an attractive fuel cell performance, attaining an output of 1764 mW cm⁻² at 700 °C and operating for more than 200 h. Manipulation of Nb-doped SrFeO_{3-δ} can be seen as a “one stone, two birds” strategy, enhancing cathode performance while retaining good stability, thus providing an interesting approach for constructing high-performance cathodes for H-SOFCs.

Biography:

Hailu Dai, PhD degree, major in materials science, is now an associate professor and master tutor of the School of Materials Science and Engineering of Yancheng Institute of Technology. Dr. Dai is mainly engaged in the research of solid oxide fuel cells, especially in the proton conductor fuel cell cathode material performance improvement. She has published more than 30 SCI papers, including 2 ESI highly cited papers, 1 ESI hot spot paper.

Developing Nanomaterials and Electrolyser Systems for Power to X Applications

Dr. Rahman Daiyan^{1*}, Scientia Prof. Rose Amal², Dr. Josh Leverett¹, Dr. Zhipeng Ma², Putri Ramadhany²

¹School of Minerals and Energy Resources Engineering, UNSW Sydney, Sydney, NSW 2052, Australia

²School of Chemical Engineering, UNSW Sydney, Sydney, NSW 2052, Australia

Abstract:

Electrochemical approaches to closing both the carbon and nitrogen cycles have emerged as promising routes towards decarbonization of the world economy, and a shift towards energy

sustainability and enabling a circular economy. The electrochemical reduction reaction of CO₂ (CO₂RR) and nitrates/nitrites (NO₂RR) powered with renewable electricity provides a pathway for simultaneously alleviating their expulsion into the environment, whilst converting intermittent renewable energy to value-added and stable chemical commodities (through a renewable Power-to-X platform). Recently, simultaneous CO₂RR and NO₃RR has also been employed to synthesize C-N products such as urea, amines, and amides, demonstrating the capability to decarbonize fertilizer, fine chemicals, and pharmaceutical industries.

Our research focuses on focuses on the design, synthesis, and application of highly active nanomaterials for various energy conversion reactions. For example, our transition metal and carbon-based single atom catalysts (SACs) exhibit low cost, minimal metal usage, and excellent activity facilitated by large surface areas and exposure of active sites. By tuning the coordination structure of these single atom catalysts, we demonstrate structure-activity correlations for (i) the electrochemical conversion of CO₂ to CO and syngas, (ii) the electrochemical conversion of nitrates to ammonia, and (iii) simultaneous CO₂ and NO₃⁻ conversion to urea. Our metal-based catalysts have also been employed for C-N coupling; using *p*-block metal oxides (BiO_x and SnO_x) and a CuO_x matrix to provide dual active sites for the conversion of waste CO₂ and nitrates to formamide. Finally, we design and optimise the reaction at scale, using an electrolyser setup capable of continuous reactions at high current densities.

Biography:

Dr. Rahman Daiyan is a renewable energy and powerfuel specialist with a track-record in nanomaterial and system development for energy conversion reactions. He is a Senior Lecturer and Scientia Fellow at the School of Minerals and Energy Resources Engineering at the University of New South Wales, and an ARC DECRA Fellow. He is a Chief Investigator at the ARC Training Centre for The Global Hydrogen Economy, ARC Centre of Excellence for Carbon Science and Innovation, ARENA funded HyGate project. He is the deputy-director of NSW Government funded Powerfuels including hydrogen network, comprising 70 industry partners.

Structure Design and Performance Optimization of Metal-Supported Proton Ceramic Fuel Cells

Lichao Jia^{1*}, Chenzhao Liu¹, Jian Li¹

¹Huazhong University of Science and Technology, China

Abstract:

Currently, the commercial application of Solid oxide fuel cells (SOFCs) is mainly limited by operating temperature and mechanical strength. Among various types of SOFCs, metal-supported solid oxide fuel cells (MSCs) show significant development potential, utilizing high-strength metal support structures. However, MSCs typically employ oxygen ion conductor materials as electrolytes, requiring operation at high temperature, which restricts their commercial viability. Proton ceramic fuel cells (PCFCs) use proton conductors as electrolytes and operate at temperatures below 700 °C, which allows the low-temperature operation of SOFCs. However, PCFCs often use electrodes or electrolytes as supports, and their strength is not as strong as metal supports.

To tackle the challenges related to operating temperature and mechanical strength in SOFCs, this study introduces a novel concept known as Metal-Supported Proton Ceramic Fuel Cells (MS-PCFC), combining features of MSCs and PCFCs. Notably, the thermal expansion coefficient mismatch between Ni support and the proton conductor electrolyte BaZr_{0.1}Ce_{0.7}Y_{0.2}O_{3-δ} in

MSCs poses a significant hurdle. To address this, a transition layer was developed to mitigate the expansion mismatch issue, leading to the following key findings: An 80wt% NiO-20wt% BZCY transition layer was fabricated, demonstrating effective mitigation of the expansion mismatch between Ni support and BZCY electrolyte. Utilizing Ni-supported transition layers (80wt% NiO-20wt% BZCY), anodes (60wt% NiO-40wt% BZCY), BZCY electrolytes, and a cathode material comprising $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-\sigma}$ mixed with BZCY, the MS-PCFC single cell achieved a peak power density of 0.8 W/cm^2 at 650°C .

Biography:

Dr. Lichao Jia is currently a Professor in School of Materials Science and Engineering at Huazhong University of Science and Technology (HUST). He received his PhD in Materials Science from HUST in 2012. Then he worked with Prof. Jian Li at HUST as a postdoctoral fellow until 2014, during this period he visited Curtin University, Australia and worked with Prof. San Ping Jiang for 1 year as a visiting scholar. His research interests are development of high-performance electrodes for SOFC and SOEC, combining theoretical and experimental studies.

ROOM B

Session: Sustainable Materials and Environment

Keynote Talks

The Properties of Nanobubbles and Their Applications in Sustainable Agriculture

Lijuan Zhang^{1*}, Jun Hu²

¹Shanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Science, China

²Shanghai University, China

Abstract:

Nanoscale gas bubbles are attracting increasing attentions in the past decade considering their significant applications in the field of medical health, agriculture and environmental fields, etc. They have some unique properties, such as superstability, high mass transfer efficiency, high zeta (ζ) potential and special biological effects in solution or on the surface of solid/liquid. In this presentation, those special properties will be discussed first. It was proven that nanobubbles could promote the growth of plants, fish, and mice, they also were used in the vegetable seed germination and improve of saline-alkali lands, etc. Finally, the key questions remained or prospectives are also suggested.

Biography:

Prof Lijuan Zhang, who is a supervisor of PhD students currently. She worked as a postdoctor in Max Planck Institute of Polymer research in Mainz from 2007 to 2009. Then she came back and was employed in Shanghai institute of Applied Physics of CAS. Her research mainly focuses on the fundamental properties of nanobubbles and their applications in environmental and biological fields mainly based on synchrotron radiation techniques.

Reimaging Catalyst Development for CO₂ Reduction and Hydrogen Production

Sibudjing Kawi, Kang Hui Lim*, Claudia Li and Guoqiang Song

Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 119260, Singapore

Abstract:

Traditional catalysis refers to using high-temperature furnaces to provide heat energy for chemical transformations governed by thermodynamics and kinetics. With the ongoing push for better and more efficient catalytic processes, unconventional routes employing non-isolated thermal effects, such as solar (i.e., photo(thermal)catalysis) and plasma, have helped catalysis achieve new heights. Here, we introduce the latest catalytic developments we have developed, including advanced core-shell morphology, defect engineering that can enhance photo(thermal) effects via effective light harvesting, photoinduced hot electrons and localized heating. The potential of photothermal catalysis was demonstrated in several green reaction-based applications, such as catalytic methane decomposition, dry reforming of methane, CO₂ reduction reactions. Due to plasma technology's intrinsic non-equilibrium nature, enhanced catalyst properties with plasma treatment and new possibilities via in-plasma catalysis configuration have helped produce desirable products efficiently. We demonstrated that the creation of abundant OH⁻ and enhanced H₂ spillover effect were enabling features endowed to a catalyst for effective CO₂ reduction. More importantly, plasma catalysis using dielectric barrier discharge (DBD) allows for low (ambient) temperature reactions, which allow active metal species, including single atomic centers, to remain stable. The stability is attributed to the prevention of the sintering effect, which is typically accelerated at higher temperatures. Consequently, our developed Pt single-atomic catalyst in non-oxidative coupling of methane gave a superior selectivity towards C₂ formation due to disfavored deep dehydrogenation on single Pt sites. Lastly, catalytic reactions can innovatively be combined with stable membrane technology, to give improved activities with facile and instant removal of desirable products sustainably.

Biography:

A/Prof. Sibudjing Kawi did his Bachelor, Master, Ph.D. and Postdoc at Univ. Texas (Austin), Univ. Illinois (Urbana-Champaign), Univ. Delaware, and Univ. California (Davis) before he joined National University of Singapore. His research focuses on the development of nanostructured catalysts (for thermal, plasma, photo, electro, photo-thermal catalysis) coupled with ceramic hollow fiber membranes (zeolites, perovskites, MOFs, Pd-alloys, composites) for CO₂ capture & utilization and hydrogen production & separation. He has published > 450 papers (citations > 26,500, h-index = 87). He has been the World's Highly Cited Researcher by Clarivate since 2021.

Designing New Materials for Sustainable Technologies

Michelle J.S. Spencer^{1*}

ARC Centre of Excellence in Future Low-Energy Electronics Technologies, School of Science, RMIT University, GPO Box 2476 Melbourne Victoria, 3001, Australia

Abstract:

Our society is heavily reliant on electronic devices to power many of our everyday items, such as mobile phones and computers, as well as being essential for industrial processes.

However, these devices often consume significant amounts of energy and are reaching their limits. New materials are needed to provide renewable energy storage solutions and low power electronics. In this talk I will discuss examples where we used density functional theory calculations and ab initio molecular dynamics simulations to develop new materials for rechargeable batteries and for components in electronic devices. I will focus on the outcomes of the following projects: 1) Tuning the mechanical, chemical, and piezoelectric properties of 2D materials; 2) van der Waals heterostructures for multiferroics; and 3) Modified electrolytes for Li-metal batteries. References: ACS Appl. Nano. Mater. 6 (2023) 14767; J. Mater. Chem. C 11 (2023) 666; Mater Today 44 (2021) 69; J. Phys. Chem. C 124 (2020) 24391; Nanoscale 14 (2022) 4114; J. Mater. Chem. A 10 (2022) 13254; Chem. Eur. J. 27 (2021) 12826; Batter. Supercaps 4 (2021) 1126; Nanomaterials 11 (2021) 2391; Surf. Interfaces 22 (2021) 100836.

Biography:

Professor Michelle Spencer leads the Computational Materials Chemistry group at RMIT. She is Deputy Director of the STEM Centre for Digital Innovation, former Associate Dean of Applied Chemistry & Environmental Science, and a Centenary Fellow of the RACI. She has published over 130 refereed publications and has received numerous awards for her research and teaching. She is a Research Associate Investigator in the ARC Centre of Excellence in Future Low-Energy Electronics Technologies and has been awarded grants from the Australian Research Council (ARC), the Australian Renewable Energy Agency (ARENA), the Australian Government and Industry.

Microwave Responsive Catalysts: Coupling Reaction and External Fields for Improved Energy Efficiency

Jiahua Zhu^{1*}, Tuo Ji¹, Minjiao Chen¹

¹Nanjing Tech University, China

Abstract:

Microwave, a type of electromagnetic wave, is well known for its cooking function. Though industrial applications of microwave have been reported in drying, metallurgy and digestion, the thermal and non-thermal effects of microwave is still an ongoing debate in the field. In other words, the function of microwave could be far beyond heating. Specifically, in multiphase reaction systems, microwave fields produce complex polarization phenomena, which greatly changes the interfacial interaction and dynamical adsorption/desorption of fluid molecules in forms such as polarization, rotation and vibration, resulting in sharp transition from equilibrium to non-equilibrium states in terms of transport and reaction at localized micro-interfacial domains. Such non-thermal effect of microwave in multiphase reaction systems would generate a series of abnormal or unexpected phenomena and thus has great potential to generate significant impacts in future industrial electrification processes. In this talk, a new family of structural catalysts with microwave responsive capability, named "Microwave Responsive Catalysts (MRC)" will be covered which breaks through the energy efficiency limitation of biomass conversion reactions. MRC is responsible for microwave absorption, heat generation, and catalytic reaction, the energy efficiency of reactions could be dramatically improved benefiting from the spatial alignment of the thermal field and reaction field. In sum, these materials demonstrated great potential to serve as an electrification tool in future chemical engineering processes under the climate of carbon neutralization.

Biography:

Dr. Jiahua Zhu is now a professor and vice dean of Chemical Engineering at Nanjing Tech University. He worked at the University of Akron in 2013 as Assistant Professor and he was early promoted to Associate Professor in 2018. Dr. Zhu's current research interest covers the biomass-derived advanced materials and biomass conversion. Dr. Zhu has coauthored >180 peer-reviewed articles, four book chapters. He was awarded the Young Leader Development Award from Functional Material Division of The Minerals, Metals & Materials Society, Early Career Award from Polymer Processing Society and Early Career Investigator Award from ECS Electrodeposition Division.

Fabrication of Three-Dimensional Graphene for Advanced Oxidation

Hongqi Sun*

School of Molecular Sciences, The University of Western Australia, Perth, WA6009, Australia

Abstract:

Water pollution has attracted much attention due to the ever-increasing water scarcity. As one of most promising technologies, advanced oxidation processes (AOPs) have been extensively studied. Recently, sulfate radicals based AOPs (SR-AOPs) have been explored because of their high oxidation potential, flexibility to a wide pH range, and feasible process free of metal leaching and sludge. Metal-free catalytic oxidation can further advance this technology. For example, graphene, carbon nanotubes, and nanodiamonds can efficiently catalyse the process and at the same time, will avoid the metal leaching from the beginning. Sometimes the separation of nanostructured materials can be an issue for potential practical applications, thus this talk discusses the fabrication of macroscopic metal-free materials for SR-AOPs. Three-dimensional (3D) nitrogen-doped reduced graphene oxide beads (NrGO_b) were synthesised via a self-assembly method and then applied in heterogeneous activation of peroxymonosulfate (PMS) for the oxidation of hydroxybenzoic acid (HBA). Moreover, macro cubes were also synthesised by a simple cross-linking and thermal annealing procedure, after which they were employed in the activation of peroxydisulfate (PS) for the degradation of sulfamethoxazole (SMX). The catalysis mechanism and degradation pathways will also be discussed.

Biography:

The speaker is the University Professor of Chemistry in School of Molecular Sciences at The University of Western Australia (UWA), Australia. He is a current member of the ARC College of Experts, Delegate to the Australia-USA Hydrogen Research Partnerships, and Board Director at MIRWA. His research focuses on novel energy catalysis and environmental remediation. He has published over 300 journal papers, with > 35,000 citations and an H-index of 104. He has been a Highly Cited Researcher since 2019, and was named Top 40 Australian Research Superstars (The Australian, 2020), and 2023 WA Mid-Career Scientist of the Year.

Green Roof Systems and Building Facades - Absorption, Scattering, and Diffusion Coefficients of Vegetation

António Tadeu^{1,2*}, João Carrilho¹, Andreia Cortês^{1,3}, João Almeida^{1,3}

¹Itecons, Coimbra, Portugal; ²University of Coimbra, CERIS, Department of Civil Engineering,

Coimbra, Portugal;³University of Coimbra, CERIS, Coimbra, Portugal;

Abstract:

Vegetation in green roof systems and building facades can contribute to sustainable urban planning, reducing sound level and absorbing sound energy. These positive contributions depend on the growing media (soil), the plant type (leaf, stem, and root), and vegetation coverage.

This work reports a set of experimental measurements carried out in a reverberation room and in an anechoic chamber to assess the effect of the plant type and vegetation coverage on the sound absorption, diffusion, and scattering properties.

It first describes the experimental setups and characterizes the plants and soil used. Then, it analyses the results to evaluate the contribution of each or combined components.

Acknowledgements:

This work is part of the research activity carried out at Civil Engineering Research and Innovation for Sustainability (CERIS), funded by FCT under project UIDB/04625/2020.

Biography:

Ph.D. in Civil Engineering from the Massachusetts Institute of Technology (MIT), Full Professor at the Department of Civil Engineering of the University of Coimbra. President of the board, technical and scientific supervisor, and R&TD Unit coordinator at Itecons. Editorial Board Member for International Magazines (Computer Modelling in Engineering & Sciences, Engineering Analysis with Boundary Elements; Revista Internacional Construlink RIC). Has published 4 books and more than 200 papers in peer-reviewed international scientific journals in the research areas of numerical modeling, experimental and analytical studies of heat transfer, and acoustic wave scattering.

Single-Atom Catalysis for Advanced Water Decontamination

Xiaoguang Duan*

School of Chemical Engineering, The University of Adelaide, Australia

Abstract:

A universal principle for advanced catalyst design is precisely tailoring favourable active sites with optimal geometric and electronic properties toward target reactions.¹ Homogeneous catalysts demonstrate excellent activities and selectivity because of the well-defined catalytic sites and tuneable coordination structures; however, these catalysts are typically of poor stability and recyclability. In recent studies, the downsizing metal species into isolated single-atom metal sites in supporting materials are appealing in catalysis, defined as single-atom catalysts (SACs).²⁻⁴ The locally confined single metal atoms are polarised and no metal-metal bonds form in the SAC structures. Due to the mononuclear nature of the catalytic sites, SACs attain the maximum atomic utilisation efficiency and exhibit exceptionally high catalytic activities and selectivity in many fine-chemical synthesis.¹ SACs also display superior structural robustness and stability over their bulky or nanoparticle counterparts due to strong covalent binding between the single metal sites and the supports.

In this work, we developed a series of structure-well-defined carbon-based single-atom catalysts (SACs) to replace conventional metal counterparts and drive several key processes

in advanced oxidation processes (AOPs) for the purification of organic contaminants in wastewater. These materials are featured by the mass synthesis procedure from low-cost precursors and high performance in catalysis. We found that SACs can effectively activate various peroxides to generate reactive oxygen species (ROS) and decompose organic contaminants in water via radical and nonradical pathways. We used both advanced characterisation techniques as well as density functional theory calculations to reveal the molecular/coordination structure of the derived SACs, featured electronic structures, as well as relations with the catalytic behaviours in AOPs. The activation of peroxides and evolution of reactive oxygen species are identified by a diversity of experimental and analytical methodologies. The SAC catalysts demonstrate great activity and stability in long-term operation with regulated redox capacity to oxidize a diversity of micropollutants. Outcomes will advance the water purification technologies using green and cutting-edge SAC-based oxidation technology to secure water safety in the post-COVID era.

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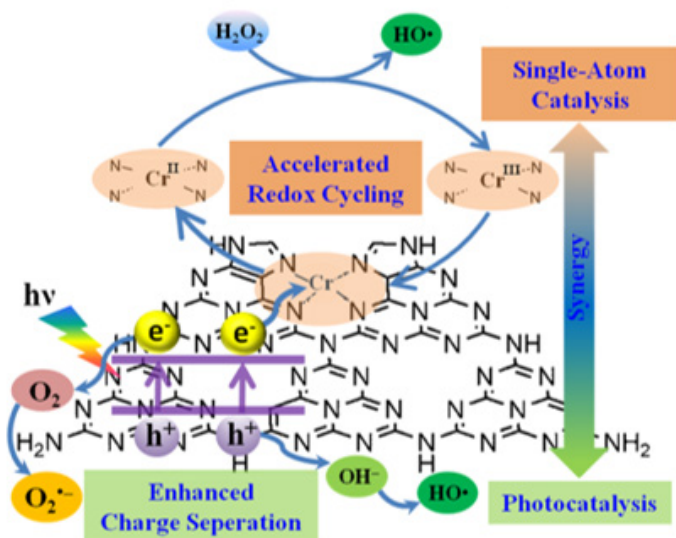


Figure 1. Single atom catalysts for catalytic evolution of reactive species for water purification.

Biography:

Dr. Duan is an Associate Professor and ARC Future Fellow at School of Chemical Engineering

of UoAdelaide. He also serves as the Discipline Lead of ChemEng and Deputy Director of Research in the school. 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 (one DECRA, 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 86 and a total of 26,000 citations (Web of Science). He was recognized as a Global Highly Cited Researcher in Environment/Ecology and Chemistry in 2022 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.

Invited Talks

2D Nanosheets Based Membrane for Fast Wastewater Treatment

Cheng Chen^{1*}, Wenjin Geng¹, Xinxin Ye¹

¹*School of Resources and Environment, Anhui Agricultural University, 130 Changjiang West Road, Hefei, 230036, Anhui, China*

Abstract:

Membrane separation has attracted tremendous attention for its vital role in providing clean water and a sustainable environment as a cost-effective and energy-efficient technique. The two-dimensional (2D) nanosheet-based membrane presents the potential to tackle the trade-off between permeance and rejection ability compared to the conventional organic polymeric membrane. However, the inevitable polarization effect of solute concentration on the membrane surface challenges the membrane for practical application. An effective in-situ catalytic degradation of the solute should be a new trial to decrease the polarization effect during the solute travel through the 2D nanosheet-based membrane. More importantly, the nanoconfined active sites further produce extra nanochannels for solvents passing through. We previously studied boron nitride, MXene, and graphene oxide membranes for clean water, yet the limit of these 2D nanosheet-based membranes is still in the infancy stage.

In this oral presentation, we would like to show some recent results based on the 2D nanoconfined catalytic membrane for organic dye and antibiotic removal from the simulated aquatic environment. The improvement in simultaneous permeance and separation ability further brings the 2D nanosheet-based membrane a step closer to practical application.

Biography:

Professor Cheng Chen obtained PhD from the Institute for Frontier Materials (IFM) at Deakin University in 2020 before starting his independent research at Anhui Agricultural University (AAU), where he led the lab of 2D Nanomaterials-Synthesis, Process and Application. During the past 10+ years, his research has focused on 2D nanomaterials, including boron nitride, graphene, MoS₂, and MXene. Based on the previous work, 2D nanomaterials have been developed for clean water and energy (Nature Communications 9.1 (2018): 1902; npj Clean Water 6.1 (2023): 38.); Joule 4.1 (2020): 247-261; Advanced Energy Materials 10.18 (2020): 1904098.).

Exploration of C–N Coupling for Electrocatalytic Urea Synthesis

Junxian Liu^{1*}, Yuantong Gu¹, and Liangzhi Kou¹

¹*School of Mechanical, Medical and Process Engineering, Queensland University of Technology, Brisbane QLD 4001, Australia*

Abstract:

Electrocatalytic coupling of N₂ and CO₂ into urea under mild conditions is a promising approach to reducing energy consumption and environmental pollution associated with the conventional Haber-Bosch process. However, the existing method suffers from the extremely low reaction efficiency due to the sluggish C–N coupling and the low selectivity for urea formation. Here, two novel mechanisms for high-efficiency urea production from N₂ and CO are proposed based on density functional theory (DFT) calculations. In the first mechanism, we proposed a potential pathway involving the N–N bond breakage to facilitate the subsequent C–N coupling. Interestingly, the inert N≡N bond of the adsorbed *N₂ can be gradually weakened and eventually broken through two protonation steps, leading to the facile CO adsorption on the dissociated *NH and the effortless C–N coupling to form the urea precursor *NHCONH. The second mechanism suggests a promising route for urea production from N₂ dimerization and CO, where C–N coupling can be achieved without breaking the N–N bond. Additionally, a simple descriptor, namely, effective d electron number, which merely consists of intrinsic properties of the catalysts, is constructed to quantitatively describe and predict the electrocatalytic urea activity of dual-atoms catalysts. Our work offers new opportunities to advance the rapid discovery of novel mechanisms and efficient catalysts for electrochemical synthesis of urea.

Biography:

Dr Junxian Liu received her Ph.D. degree in 2022 from Griffith University and Master degree in condensed matter physics from Shanghai University in 2017. She has been a postdoctoral research fellow at Queensland University of Technology since 2022. Her current research mainly focuses on computational materials for high-performance electrocatalysts.

Greening the Catalyst Landscape: Basalt Fiber-Supported Ni/LTA Catalysts for Hydrogen Production and Carbon Nanotube Synthesis

Claudia Li*, Guoqiang Song, Kang Hui Lim, Sibudjing Kawi

Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 119260, Singapore

Abstract:

In the pursuit of sustainable energy solutions, catalytic methane decomposition (CDM) emerges as a promising pathway for hydrogen (H₂) gas production and the synthesis of valuable carbon nanotubes (CNTs). However, challenges persist in achieving stability in gas-to-solid reactions, often hindered by limitations in CNT growth and reactor volume constraints. This study introduces a groundbreaking approach by employing eco-friendly basalt fiber-supported Ni/LTA catalysts, incorporating the use of green materials and a non-template method in LTA zeolite synthesis. These innovative catalysts not only ensure CO_x-free H₂ generation but also exhibit an exceptional 3.7-fold extension in CDM reaction times. Operating at 500 °C, the basalt fiber-supported catalysts deliver an impressive H₂ production rate of 3.1 mol g_{Ni}⁻¹ h⁻¹ over 22 hours, outperforming Ni/LTA nanopowder counterparts.

Moreover, the catalysts showcase uniform and robust CNT growth, along with sustained and stable H₂ generation lasting up to three times longer than traditional CDM catalysts reported in the literature. The integration of flexible basalt fiber catalysts into an H₂-permeable LTA-Pd membrane reactor further enhances the green approach, with a 36% increase in reaction time and a 40% boost in CH₄ conversion. Achieving up to 45% CH₄ conversion over 27 hours, surpassing expected equilibrium conversion rates, marks a significant stride towards sustainable H₂ production. This transformative study not only propels the development of functional catalyst materials but also sets the stage for environmentally conscious thermocatalytic processes, reinforcing the importance of green materials in advancing the energy landscape.

Biography:

Dr. Claudia Li received her Ph.D. from Swinburne University of Technology in 2021. Her Ph.D. work was focused on the development and simulation of oxygen permeation fluxes through carbon dioxide-resistant dual-phase mixed ionic-electronic conducting (MIEC) membranes. She was awarded the Swinburne's competitive Deputy Vice Chancellor (DVC) Travel Award, which supported her research attachments to Curtin University in Australia and then to Tiangong University and Shandong University of Technology in China. She is presently working as a Research Fellow at the National University of Singapore on the development of novel multi-layered catalytic hydrogen permeable membranes for methane decomposition.

Green Future or Emerging Contamination of Nanoplastic: How to Know?

Xian Zhang^{1*}, Théogène Habumugisha¹, Zixing Zhang¹

¹Key Lab of Urban Environment and Health, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, P.R. China

Abstract:

We developed a novel method utilizing matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) for polystyrene nanoparticle characterization, exploiting periodic and equispaced fingerprint peaks (104 Da) corresponding to the styrene monomer's molecular weight. The method exhibited a detection limit of 0.05 µg/g. Validation involved investigating polystyrene nanoparticle bioaccumulation and biodistribution in zebrafish tissues following exposure to varying polystyrene nanoparticle concentrations (1-20 mg L⁻¹) for 20 days. polystyrene nanoparticle presence was confirmed in zebrafish tissues, with the highest accumulations observed in the intestine, liver, and gill (275.01, 260.32, and 215.16 µg g⁻¹ wet weight, respectively) and the lowest in muscle and brain (85.71 and 58.23 µg g⁻¹ wet weight, respectively). Uptake kinetics indicated longer saturation times for tissues exposed to lower concentrations (1-5 mg L⁻¹) compared to higher concentrations (10-20 mg L⁻¹). These findings are crucial for understanding polystyrene nanoparticle fate and for assessing environmental and ecological risks associated with plastic nanoparticles.

Biography:

Professor Dr. Xian Zhang, from the Institute of Urban Environment, Chinese Academy of Sciences, specializes in environmental chemistry and toxicology. Her research interests include the environmental behaviors of emerging pollutants such as environmental estrogens, brominated flame retardants, pharmaceuticals and personal care products

(PPCPs), nanoparticles, and microplastic particles. She focuses on the transportation and transformation of nanoparticles in the food chain, including processes such as bioaccumulation, depuration, and metabolism.

Potential Use of Biomass Ash to Contribute to Reduce CO₂ Emissions in the Construction Sector

Wesley B. S. Machini^{1,2}, João A. S. Almeida^{1,2}, Julieta M. P. António^{2,3*}

¹University of Coimbra, CERIS, Coimbra, Portugal; ²Itecons - Institute for Research and Technological Development in Construction, Energy, Environment and Sustainability, Portugal; ³University of Coimbra, CERIS, Department of Civil Engineering, Portugal.

Abstract:

The construction sector is responsible for intensive energy consumption and a release of large CO₂ emissions worldwide. Meet the cement demands and at the same time reduce CO₂ emissions is a huge challenge that the sector faces. This paper aims to characterize a biomass ash from two Portuguese biomass plants, which incinerate wood waste, such as pine and eucalyptus chips, in order to evaluate its potential as partial substitute for cement. The biomass ash was characterized in terms of physical, mineralogical and chemical properties, including the evaluation of leaching behavior, pozzolanic activity and hydration heat. The mechanical properties were analyzed through compression and flexural strength tests of hardened mixes of ash, cement and sand, at the age of 28 days and 90 days. Cement replacement percentages of 5%, 15%, 25% and 50% were investigated. The activity index of this biomass ash did not reach the values required for fly ash, according to the EN 450-1 standard. However, for 25% cement replacement, good compressive strength values of 34.8 MPa and 41.3 MPa were obtained at 28 and 90 days, respectively. Replacing 50% of cement led to low compressive strengths, below 10 MPa. This finding suggests that for large replacement percentages it will be necessary to investigate other approaches to activate ash reactivity for improving its binding properties.

Acknowledgements:

This work is part of the research activity carried out at Civil Engineering Research and Innovation for Sustainability (CERIS), funded by FCT under project UIDB/04625/2020.

Biography:

Julieta António is PhD in Civil Engineering from the Faculty of Sciences and Technology, University of Coimbra, Portugal. She is Associated Professor at the University of Coimbra and her teaching activities include courses in the areas of Acoustics, Sustainability and Mechanics. Her areas of research interest are Building Sciences, Construction Sustainability, Wave propagation, Acoustics, Boundary Element Method and Meshless Methods.

Session: Australian-Korean Workshop on Energy Materials

Interfacial Materials Engineering for Scalable Transparent Organic Photovoltaics

Dong Chan Lim^{1*}, Soyeon Kim¹

¹Nano Surface Technology Division, Korea Institute of Materials Science (KIMS), R.O.Korea

Abstract:

The interfacial layers assume a pivotal role in augmenting the performance and stability of organic photovoltaics (OPVs). Despite the attainment of high efficiency in OPVs, the challenges associated with large-scale manufacturing and the requisite nanoscale uniformity during coating have impeded widespread production. Furthermore, there exists a compelling necessity for sustained research endeavors directed at enhancing the performance of OPVs, with a specific emphasis on elevating their visible light external quantum efficiency (EQE) to ameliorate the efficiency of semitransparent OPVs (ST-OPVs). In response to these challenges, we proffer diverse conceptual frameworks, such as the utilization of bilateral self-assembled monolayers to modify the electron transport layer and/or hole transport layer, along with the incorporation of plasmonic nano-clusters and a transparent top electrode. In a recent study, the incorporation of phosphotungstic acid as an annealing-free hole transport layer (HTL) and as a solid additive into the photoactive layer (PM6:Y6:PC71BM) in conventionally structured OPVs significantly enhances the power conversion efficiency (PCE) to 17.28% and 16.33%, respectively, as compared to the reference device employing PEDOT:PSS (15.88%). Additionally, we have successfully engineered a large-area OPV module featuring an impressive PCE of 15.18% and an active area of 54 cm², attaining approximately 85% of the efficacy observed in small-area OPVs. Notably, ST-OPVs also yield noteworthy device performance and transparency, registering a PCE of 10.37% and an average visible transmittance (AVT) of 36.27% through the application of bilateral self-assembled monolayers to modify the ZnO electron transport layer in inverted OPVs.

Biography:

Dong Chan Lim received his Ph.D. degree in Cluster Physics from Konstanz University, Germany in 2007. He is a head of Nano Technology Innovation Center and principal researcher of the Energy and Electronic Materials Center at the Korea Institute of Materials Science (KIMS), Korea. His main research interests are in photovoltaics and related materials, such as quantum clusters and transparent electrodes, functional thin films. In addition, his research interests include photoelectrochemical devices and hybrid energy conversion materials to create clean and sustainable energy and water.

Highly Conductive Polymers for High Performance, Low-Cost Organic Electronics

Yong Hyun Kim^{1*}

¹Pukyong National University, Republic of Korea

Abstract:

Highly conductive electrodes based on polymers are a key component of future flexible organic devices. In the last decade, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) has been most widely used as conductive polymers, with successful commercial applications. Due to their high conductivity, chemical and thermal stability, and

superior processability, PEDOT:PSS thin-films have received much attention as alternative transparent conductive electrodes to replace indium tin oxide (ITO). We report various strategies for preparing highly conductive transparent PEDOT:PSS films. These approaches greatly improve the electrical and mechanical properties of PEDOT:PSS thin-films.

Furthermore, skin-attachable conductive materials have attracted significant attention for use in wearable devices and physiological monitoring applications. Soft and stretchable sensing systems based on stretchable conductive materials can provide a novel platform for monitoring human activities and realizing human-machine interfaces. Because intrinsically stretchable materials are highly desirable, polymers are regarded as offering unique opportunities for stretchable technologies owing to their versatility and high stretchability. Here, we demonstrate highly robust, conductive, and stretchable conductive hybrid films based on PEDOT:PSS and biopolymers, prepared using a simple and low-cost approach. The conductive hybrid films offer new opportunities for fabricating stretchable electrodes and multifunctional skin-attachable wearable sensors.

Biography:

Yong Hyun Kim is a professor at Pukyong National University in Korea. He received his PhD degree from Technische Universität Dresden, Germany in 2013, under the supervision of Prof. Karl Leo. After that he worked as a post doctoral associate at University of Minnesota, and later was promoted to Professor in 2014. He joined again in IAPP as a visiting professor to take a sabbatical leave in 2019. His research focuses on conductive polymers and novel device architectures for organic electronics. He published over 90 peer-reviewed papers including his pioneering research in highly conductive polymer materials for organic optoelectronic devices.

Development of Metal Halide Perovskites for High-Performance Solar Cell and Artificial Synapse

Zitong Wang^{1*}, Lyu Miaoqiang¹, Ekyu Han¹, Bowei Zhang¹ and Lianzhou Wang¹

¹*School of Chemical Engineering and Australian Institute for Bioengineering and Nanotechnology, the University of Queensland, St Lucia, QLD 4072, Australia*

Abstract

Metal halide perovskites have emerged as promising semiconductors for optoelectronic devices due to, ease of fabrication, attractive photophysical properties, their low cost, highly tuneable material properties, and high performance. High-quality thin films of metal halide perovskites are the basis of most of these applications including solar cells and artificial synapses.[1] Herein, we aim to introduce our research progress on developing high-quality thin-films of halide perovskites and their lead-free analogues, as well as their applications in solar cells and electronic artificial synapses. A facile solvent-engineering strategy is designed for effective suppression of both surface and bulk defects for improving perovskite film quality, leading to a high efficiency of 35.99% under 1000 lux indoor light illumination. [2] Thermal evaporation represents an attractive alternative method for developing high-quality halide perovskite thin films. We synthesized the FASnI₃ perovskite thin films via a pure sequential thermal evaporation method. By exploring various deposition parameters, we achieved high-quality FASnI₃ perovskite thin films with decent efficiencies and stability in lead-free perovskite solar cells. Lastly, a two-terminal artificial synapse using silver-based perovskite-derivative CsAg₂I₃ has been demonstrated. Interestingly, we identify that addition

of small amounts of hydroiodic acid to the precursor solution leads to the anisotropic orientation of the CsAg_2I_3 crystal structure within the thin film, which is critical for maximise their performance in artificial synapse application.[3]

Biography:

Zitong Wang received his M. Eng from The University of Queensland in 2022. He is a current PhD student under supervision of Dr. Miaoqiang Lyu and Prof. Lianzhou Wang at The University of Queensland. His research interest is designing low-toxicity and stable halide perovskites for solar energy generation and conversion.

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Advanced Smart Window Technology with Dielectric/Metal/Dielectric (DMD) Electrodes and Electrochromic Innovations

Soyeon Kim^{1*}

¹Nano Surface Technology Division, Korea Institute of Materials Science (KIMS), Republic of Korea

Abstract:

This study observes into the utilization of vacuum deposition in the fabrication of Dielectric/Metal/Dielectric (DMD) structures as a promising alternative to Indium Tin Oxide (ITO) for flexible electronic applications. The unique property of Dielectric/Metal/Dielectric (DMD) structures, such as those containing MoO_3 and WO_3 , is their ability to exhibit different colors by varying the thickness of each layer making them suitable for applications in devices such as solar cells, displays and smart window application. Furthermore, the application of vacuum deposition in depositing electrochromic materials, particularly tungsten oxide (WO_3), onto flexible substrates is explored. This method demonstrates significant benefits over other deposition techniques, including improved uniformity, better control over thickness, and enhanced adherence to flexible substrates. These attributes are crucial for the development of efficient, durable, and flexible electrochromic devices. Lastly, we engineer the hybrid layer-by-layer electrochromic device by incorporating cathodically electrochromic material WO_3 with organic electrochromic material PEDOT:PSS to get a synergy that enhances overall performance. While WO_3 -based electrochromic devices are known for their high optical modulation, they suffer from slow switching times. On the other hand, PEDOT exhibits faster switching times but with relatively lower optical modulation. By integrating these two materials, the hybrid system capitalizes on the strengths of both: it achieves high optical modulation from WO_3 and faster switching times, akin to PEDOT, offering a significant improvement over devices using only WO_3 .

Biography:

Soyeon Kim received her Ph.D. degree in Chemical & Biomolecular Engineering from Yonsei University, Korea in 2017. She is a senior researcher of Energy and Electronic Materials Center

at the Korea Institute of Materials Science (KIMS), Korea. Her main research interests are in organic materials including synthesis and applications for energy and electronic devices.

Efficient Bifacial Semitransparent Perovskite Solar Cells Using Down-Conversion 2D Perovskite Nanoplatelets-PMMA Composite Film

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^b*Centre for Materials Science, Queensland University of Technology, Brisbane, QLD 4001, Australia*

Abstract:

Semitransparent perovskite solar cells (ST-PSCs) hold significant appeal for various applications in smart windows, multijunction tandem devices, bifacial and chargeable devices, etc. Unfortunately, to possess high transparency, the perovskite layer in the ST-PSCs must be kept at relatively thin (< 400 nm), which in turn causes insufficient light absorption and thus inferior device performance. Herein, a 2D perovskite nanoplatelets (NPLs)/poly(methyl methacrylate) (PMMA) composite thin layer is applied in the ST-PSCs to solve these problems. Thanks to its dual function of down conversion (DC) effect, converting high-energy UV photons into low-energy visible photons to enhance the photocurrent, and interfacial passivation, reducing the nonradiative recombination at the interface, the 2D NPLs-PMMA based devices with the different average visible transmittance (AVT) values of perovskite film demonstrate significantly improved power conversion efficiency (PCE) compared to the pristine devices, and remarkable UV stability, retaining over 77% of initial PCE after aging under continuous UV illumination for 280 h. More importantly, the full bifacial ST-PSCs using a transparent MoO₃/Au/MoO₃ rear electrode exhibited a record PCE of 14.26% and 10.65% with a whole device AVT of 19.4% and 26.9%, respectively, which are among the highest performing ST-PSCs of the kind reported to date.

Biography:

Dr. Yang Yang received his Ph.D. at School of Chemistry and Physics, Faculty of Science, Queensland University of Technology, Australia, in 2021 and M.S. from China University of Mining and Technology, China, in 2016. He currently is a Postdoc Research Fellow at Queensland University of Technology, Australia. His research topic is on the perovskite solar cells using carbon electrode, semitransparent perovskite solar cells, energy storage devices and the perovskite-based integrated devices.

Perovskite Solar Cells with Two-Dimensional (2D) Materials

Purevlkham Myagmarsereejid¹, Abdulaziz S. R. Bati^{2,3}, Selengesuren Suragtkhuu¹, Solongo Purevdorj¹, Abraham Adenle¹, Munkhjargal Bat-Erdene^{1,4} and Munkhbayar Batmunkh^{*1}

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²*Centre for Organic Photonics & Electronics, School of Chemistry and Molecular Biosciences, The University of Queensland, St Lucia, Brisbane, QLD, 4072, Australia*

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Abstract:

Organic/inorganic metal halide perovskites attract substantial attention as key materials for next-generation photovoltaic technologies due to their potential for low cost, high performance, and solution processability. Despite their great promises, perovskite solar cells do have some disadvantages such as use of expensive electrode materials, the high temperature required during production and poor operational stabilities. Two-dimensional (2D) layered nanomaterials such as black phosphorus and metal carbide MXene have shown great promise for use in a wide range of energy related applications including perovskite solar cells. The high degree of tunability in the properties of these unique nanomaterials offers an abundance of opportunities for next generation solar cells. In this talk, Dr Batmunkh will present the recent contributions he and his colleagues made to this cutting-edge research area and also highlight the future promises in this area.

Biography:

Dr Munkhbayar Batmunkh is an ARC DECRA fellow in Queensland Micro- and Nanotechnology Centre (QMNC) and a Senior Lecturer in the School of Environment and Science at Griffith University, Australia. Dr Batmunkh currently leads an active independent research group working on functional materials, solar cells, catalysis and their integrated systems. He completed his PhD study in School of Chemical Engineering at the University of Adelaide, in 2017. He obtained his 'Master of Engineering' degree from Gyeongsang National University, in South Korea in 2012. He completed his 'Bachelor of Science' degree in Chemistry at the National University of Mongolia, in Mongolia in 2010.

On-Skin Health-Monitoring Devices Using Highly Stretchable Conductive Hydrogels

Jungha Kim^{1*}, Ajeng Prameswati¹, and Yong Hyun Kim¹

¹Pukyong National University, Republic of Korea

Abstract:

Conductive hydrogels have emerged as key materials for wearable electronics, yet their adoption has been curtailed by issues like low sensitivity and slow response. This study introduces advanced poly(vinyl alcohol) (PVA)/poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) hydrogels, enhanced with NaCl post-treatment. These hydrogels boast remarkable mechanical strength, quick electrical response, and minimal hysteresis, alongside superior self-healing capabilities that enable them to recover their original properties and extend over 150% after healing. The improved performance is attributed to better intermolecular bonding between PVA and PEDOT:PSS, beneficial PEDOT chain rearrangements, and increased localized charges, making the hydrogels highly sensitive and efficient in real-time motion and muscle action monitoring with low power consumption less than 180 μ W and fast response time (0.88 seconds). This positions the PVA/PEDOT:PSS hydrogels as promising materials for wearable sensors in human activity monitoring, thanks to their robustness, stretchability, conductivity, and self-healing properties.

Biography:

Jungha Kim is currently a PhD student at the Department of Smart Green Technology Engineering in Pukyong National University. Her current research interests include conductive polymers and wearable electronic devices.

ROOM C

Session: Nanomaterials and Nanotechnology

Keynote Talks

Monomicellar Assembly to Synthesize Mesoporous Materials

Wei Li*

Department of Chemistry, Fudan University, Shanghai 200433, China

Abstract:

Mesoporous materials have large pore size (2-50 nm), high specific surface area, rich skeleton composition, adjustable geometric structure and unique nanoconfinement effect, and are a very important class of catalytic materials, which are widely used in petroleum refining, energy catalysis, fine chemical industry, environmental protection and other fields. However, the synthesis process still has problems such as insufficient efficiency and accuracy, relying on "trial and error method", and most of the prepared mesoporous materials are blocks, low utilization of active sites, and blocked diffusion mass transfer, resulting in poor catalytic performance. Starting from the construction of the basic structural units of mesoporous materials (single micellar units and functional monomers), we developed a directional assembly method with the self-assembly driving force - fine regulation of non-covalent bond interactions as the core, and created efficient mesoporous catalytic materials to solve the key scientific problems faced in their preparation and catalytic applications. Recent progresses will be also discussed briefly.

Biography:

Wei Li, Yangtze River Scholar Distinguished Professor at Fudan University. He obtained his bachelor degree from Heilongjiang University, doctor degree from Fudan University, China in 2008 and 2014, respectively. From 2014 to 2016, he worked as Postdoctoral fellow in University of Toronto, Canada, and Institute of Basic Sciences, Republic of Korea, respectively. After returning to Department of Chemistry of Fudan University, he became an associate professor in 2016 and a full professor from 2019 to now. He has published more than 180 SCI papers in Nature Protoc., Nature Commun., Sci. Adv., J. Am. Chem. Soc., Angew. Chem. Int. Ed., Adv. Mater., Natl. Sci. Rev., etc., which have been cited more than 20,000 times. H-index 70. He has won the first prize of the National Natural Science Award in 2020 (the second complete adult). He is currently a member of the International Mesostructured Materials Association, the Energy Chemistry Committee of the Chinese Chemical Society, and a member of the editorial working group of National Science Review.

Self-Sensing Graphene/Cementitious Concrete: A Pathway toward Intelligent Infrastructure

Yipu Guo, Wengui Li*

Centre for Infrastructure Engineering and Safety, School of Civil and Environmental Engineering, The University of New South Wales, NSW 2052, Australia

Abstract:

Conductive carbon nanomaterials have been extensively developed for smart cementitious composites to gain multifunctionalities (e.g. self-sensing, self-healing, self-heating, and electromagnetic interference shielding). This paper critically reviewed dispersion and percolation of 0-dimension (0D), 1 dimension (1D) and 2 dimensions (2D) carbon materials used in cementitious composites and their effects on the electrical and piezoresistive performances. The different dispersion methods summarized are from mechanical dispersion, ultrasonic and high shearing, chemical modification, mineral additives, to carbon materials at multiple dimensions and hybrid dispersion methods. The electrical resistivity and piezoresistivity of cementitious composites with single carbon material or hybrid carbon materials are comprehensively analysed and compared in terms of efficiency and self-sensing mechanism. Furthermore, the existing theoretical modelling studies have been reviewed, indicating that many factors related to the electrical and piezoresistive behaviours, such as water content and nanocomposite agglomeration, have not been considered yet. Although some previous studies demonstrated the potential of applying conductive cementitious composites for self-sensing or heating pavements, further explorations still should be conducted on sustainable and economical manufacturing. Subsequently, the challenges and perspectives of the self-sensing stability, data acquisition system and sensor configuration are proposed with potential solutions for future smart infrastructure.

Keywords: Carbon nanomaterials, Cementitious composite, Electrical resistivity, Piezoresistivity, Microstructure, Smart concrete

Design and Fabrication of Oxide Nanostructures on Metallic Foils via Thermal and Anodic Oxidation for Heavy Metal Mitigation

Wai Kian Tan*

Institute of Liberal Arts & Sciences, Toyohashi University of Technology, Japan

Abstract:

Heavy metal discharge through wastewater has been a matter of alarming concern. Hexavalent chromium, Cr (VI) is commonly used in the chrome plating industry and is extremely toxic and hazardous to human beings. Therefore, it is imperative to reduce the concentration of Cr (VI) in wastewater prior to its release into the environment. The World Health Organization has recommended that Cr (VI) concentrations in water should be within 0.05 mg/L. For the removal of Cr (VI), various methods can be used such as chemical precipitation, adsorption, ion exchange and photoreduction. Metal oxides in the form of powder or nanostructures formed on substrate are used for the removal process. However, although oxide powders possess higher surface area for reaction, their recovery after removal process often remains a challenge. One alternative is to use metal oxide nanostructures formed on substrate, therefore, there is a need for a rapid process that enables the fabrication and design of nanostructured oxide for efficient removal of heavy metals. In this talk, a controlled formation

of metal oxide nanostructures on metallic foils, with a rather good scalability via thermal or anodic oxidation will be presented. A controlled fabrication of metal oxide nanostructures (iron oxide, niobium pentoxide etc.) will be introduced using the abovementioned methods. Their material properties and Cr (VI) removal performances via either adsorption or photoreduction will also be discussed.

Biography:

Wai Kian Tan is currently an Associate Professor in the Institute of Liberal Arts & Sciences of Toyohashi University of Technology (TUT), Toyohashi, Aichi, Japan. His research interests and specialties are in the development of ceramic composite materials, advanced functional oxide materials, hybrid materials and renewable energy materials. Dr. Tan has published 140 peer-reviewed publications and 9 book chapters and is committed to SDGs. In a citation metric (Science-Metrix classification carried out by Elsevier for 2022), his works and collaborative researchers are ranked in a percentile rank of 2% or above in the sub-field.

Controllable Fabrication, Properties and Engineering of Green Polymer Nanocomposite

Haihua Wang*

Shaanxi University of Science & Technology

Abstract:

In this seminar, I will briefly discuss my groups' motivations, research overview and main achievements in the following three topics: (1) Low-cost, environmental and high-performance polymer nanocomposite coating for paper, wood, metal surface protection; (2) Controllable polymerization method to fabricate high-performance polymer and polymer nanocomposite; (3) Molecular design and chemical modification to enable multifunctional characteristics and performance. Our group has devoted most of time to polymer as a material platform for designing new structures to manipulate the properties with end applications in coating, surfactant, additive, oilfield, pollutant monitoring, solid electrolyte and electrode materials, etc.

Biography:

Haihua Wang is a distinguished professor in College of Chemistry and Chemical Engineering, Shaanxi University of Science and Technology. She finished her post-doctoral fellowship at the University of New Brunswick in Canada, followed by visiting professor at Bath University in UK, visiting professor at Northwestern University in US, and research professor at Korea University in Korea. She has been leading a group of Chemistry & Technology for Functional Polymer Materials in Shaanxi University of Science and Technology. She published 37 authorized patents and 138 papers. She won lots of esteemed honor/prizes including the Youth Changjiang Scholar, Korean Brain Outstanding Inviting Scientist, Distinguished Young Scholar of Shaanxi Province, Top Youth Talent award, Outstanding Young Research Award in Chemistry, New Star Award on Youth Science and Technology from Shaanxi Province, the First Prize of Provincial Science and Technology Award, the Second Prize of Provincial Patent Award, and the First/Second Prize of Technological Invention Award from China National Light Industry Association, etc. She has conducted around 20 projects until now and kept up with good collaborations with large-scale Chinese companies, including Chengdu Banknote Printing Company, PetroChina Changqing Oilfield Company, Shaanxi Baotashan Paint Co. LTD, Shaanxi Yanchang Petroleum (Group) Co. LTD and so on. Many technologies which she

invented have been successfully commercialized for the real industrial applications.

Multifunctional Epoxy/Graphene Nanoplate Composites: A Decade of Advancements

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¹STEM and Future Industry Institute, University of South Australia, SA 5095, Australia

²Department of Energy Application Engineering, Far East University, Tainan County 744, Taiwan

³College of Aerospace Engineering, Shenyang Aerospace University, Shenyang, Liaoning Province 110136, China

Abstract:

Epoxy resins, one class of the most important commercial polymers, are extensively used in various industries such as coatings, adhesives and composites. However, the application of epoxy resins is limited by unideal stiffness and inherently poor fracture toughness. Being one of the stiffest and strongest materials ever reported, graphene holds great promise as a new class of fillers for polymer processing and polymer composites. Since 2008, Ma's research team have conducted extensive research of developing graphene nanoplatelets (GNPs) and using them for processing of epoxy, elastomers and conducting polymers. A GNP is defined as stacked graphene with an average thickness below 10 nm. GNPs exhibit a Raman I_d/I_g ratio of 0.07, which corresponds to an electrical conductivity of 1456 S/cm, as measured by a four-probe method for a film of ~10 micron in thickness.

A hardener, 4,4'-diaminodiphenylsulfone (DDS), was used to chemically modify GNPs for covalently bonding with an epoxy matrix. The interface-modified composite at 0.489 vol% of GNPs demonstrated an eight-order reduction in resistivity, a 47.7% improvement in modulus and 84.6% in fracture energy release rate. When GNPs were reacted with a long-chain surfactant, the surfactant created molecular entanglements with the matrix, resulting in composites that had an electrical percolation threshold of 0.25 vol%. The new trend is to develop new greener methods for polymer/GNP composites.

Biography:

Prof. Jun Ma's research focuses on the development of applied functional (nano)composites through processing engineering materials with a range of cost-effective, safe nanomaterials, aiming to engage with industry in the design, development and manufacturing of advanced composite materials. Prof. Ma is the founder and the Editor-in-Chief for an academic journal Advanced Nanocomposites.

To-date Prof. Jun Ma as the lead Chief Investigator has attained a research income of \$2.6 million; his total research income is over ten million dollars. Prof. Ma has been appointed to the ARC College of Experts since 2022.

Defect Engineering in Accelerating Charge Separation and Transfer in Photoelectrochemical Water Splitting

Zhiliang Wang*

School of Chemical Engineering, University of Queensland

Abstract:

The photocatalysis and photoelectrocatalysis are regarded as the dreaming technology to achieve green and sustainable chemical conversion driven by solar energy. The development of effective semiconductor catalysts is the cornerstone for achieving highly efficient solar conversion process. Defect engineering represents as a very promising strategy in accelerating the solar conversion process since it can significantly affect the charge separation and transfer (CST) in the semiconductor photoelectrodes. Herein, some typical defects, including the doping strategies and lattice distortion, will be discussed in accelerating the CST process. Especially, the machine learning was applied in investigating the doping effect in photoelectrode to discover the key criteria in dopant selection. In addition, the lattice distortion induce polarization is also reported to provide bulky driving force in accelerating CST in semiconductor film. Furthermore, the application of ferroelectric polarization in motivating the transfer of photogenerated charges will also be discussed.

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Biography:

Dr Zhiliang Wang is an ARC DECRA research fellow in The University of Queensland. After receiving his PhD degree from Dalian Institute of Chemical Physics in 2017, he joint Prof Lianzhou Wang's group focusing on solar driven chemical conversion processes, including water splitting, carbon dioxide fixation and methane conversion. He has accumulated rich experiences in the design of semiconductor based photocatalyst and photoelectrode and achieved over 70 publications in highly ranked journals such as *Adv. Mater.*, *Angew. Nat. Commun.*, etc. He has been awarded with the J G Russell Award by the Australia Academy of Science, ECR Research Award by UQ and other prizes.

Invited Talks

Facile One-Step Synthesis of High Metal-Loading Single-Atom Catalysts on Two-Dimensional Nitro-Oxygeneous Carbon as Efficient Electrocatalysts

Teera Butburee^{1*}, Jitprabhat Phonchai¹, Pongtanawat Khemthong¹, Poobodin Mano¹, Pongkarn Chakhranont¹, Saran Youngjan¹, Jakkapop Phanthasri¹, Supawadee Namuangruk¹, Kajornsak Faungnawakij¹, Xingya Wang², Yu Chen², Lijuan Zhang²

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²Shanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Sciences (CAS), No 239, Zhangheng Rd., New Pudong District, Shanghai 201204, P.R. China

Abstract:

Single-atom catalysts (SACs) have emerged as a new frontier of catalysis, as they can involve the merits of both homogeneous and heterogeneous catalysis altogether. However, SACs

synthesis usually relies on multiple-step processes, large solvent consumption, expensive precursors, or sophisticated instruments, which are not cost-effective or unaffordable in general laboratories. Moreover, most SACs usually have low metal loading (<4 wt.%) and those metal atoms often bury in the support media, leading to insufficient active sites for target reactions. In this work, we developed a facile one-step pyrolysis that results in SACs of transition metals with high loading (>10 wt.%) on two-dimensional (2D) nitro-oxygenous carbon support (M_1 -2D-NOCs, where $M = \text{Fe, Cu, Co, Ni, Zn, etc.}$). The method is solvent-free using low-cost precursors, and can be conducted in a muffle or tube furnace, making it repeatable and scalable in general laboratories. Due to the enriched metal active sites on the thin 2D-nanomaterial supports that promote the accessibility between the active sites and the reactants, high electrocatalytic performance is achieved, as demonstrated in oxygen reduction reaction (ORR). For example, Fe-2D-NOC showed a Tafel Slope of -40.860 mV/dec, V_{onset} of 0.985 V, and $E_{1/2}$ of 0.826 V vs RHE, which are nearly comparable to the benchmark catalyst (Pt/C) and among the most promising catalysts reported for this kind of reaction. The theoretical (DFT) simulation and insightful experimental characterizations were combined to study the catalytic behaviors at the active sites of these catalysts.

Biography:

Teera Butburee is currently a senior researcher at National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency (NSTDA). He received his Ph.D. from School of Chemical Engineering and Australian Institute for Bioengineering & Nanotechnology (AIBN), the University of Queensland, Australia, and B.Sc. from Department of Chemistry, Faculty of Science, Khon Kaen University, Thailand. His research interests include carbon capture and utilization (CCU), solar-harvesting technologies, catalysis, biorefinery, and nanomaterials.

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

Juan Bai^{1,2}, and Ziqi Sun*^{1,2}

¹School of Chemistry and Physics, Queensland University of Technology, 2 George Street, Brisbane, QLD 4000 Australia

²Centre for Materials Science, Queensland University of Technology, 2 George Street, Brisbane, QLD 4000 Australia

Abstract:

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

expected that this work sheds light on the enrichment of metal active sites via activating inert metal sites on oxide catalysts for boosting electrocatalytic properties.

Biography:

Juan Bai is currently a Lecturer/DECRA Fellow in the School of Chemistry and Physics at Queensland university of technology. She received his PhD degree from the Shaanxi Normal University in 2019. Her research interest mainly focuses on the design and synthesis of functional nanostructured catalysts for electrochemistry and energy conversion devices.

Ligand Mediated Surface Engineering of High-Performance Quantum Dots

Dechao Chen^{1*} and Qin Li¹

Queensland Micro- and Nanotechnology Centre, Griffith University, Brisbane, QLD 4111, Australia

Abstract:

Ligand mediated surface engineering is a powerful approach to manifest the physical and chemical properties of quantum dots. We present a general top-down and bottom-up method to attract high-quality carbon dots from crude biomass with surface ligand-induced dual emission through a colloidal synthesis strategy. The colloidal synthesis improved the quality of carbon dots in its size control and uniformity. The colloidal carbon dots showed the improved quantum yield and surface passivation induced dual emission. The results revealed the surface function and interactions. Benefitting from the good optical and colloidal stability, the colloidal carbon dots demonstrated excellent potential in large volume applications such as OLED and optoelectronic devices.

Biography:

Dr. Dechao Chen is a research fellow in the Queensland Micro- and Nanotechnology Centre (QMNC) at Griffith University. He received PhD in Chemistry from Curtin University in 2020. His research focuses on the colloidal synthesis of quantum dots including carbon quantum dots, semiconductor quantum dots and perovskite quantum dots, with addressing in the energy conversion applications in photocatalysis and optoelectronics.

Session: Green Process for Resource Recovery

Keynote Talks

A Facial Method for Preparing Battery-Grade Iron Phosphate from Iron Phosphate Residue (IPR)

Shili Zheng^{1*}, Ying Zhang^{1*}, Xiaojian Wang¹, Shan Qiao¹, Wenbo Lou¹

¹Institute of Process Engineering, Chinese Academy of Sciences, China

Abstract:

Recycling end-of-life lithium-ion batteries, including the spent lithium iron phosphate (LiFePO₄, LFP) battery, has been a hot topic with the development of electric vehicles. The recycling of Li element from the spent LFP black powder through hydrometallurgical leaching using sulfuric acid and hydrogen peroxide has been industrialized. However, the valuable

elements of Fe and P in the residue after lithium extraction are hard to recycle, restricted by the difficulty of purifying the iron phosphate. Our research group proposed a facial method for preparing battery-grade iron phosphate from the IPR. The IPR was leached with the sulfuric acid solution, and 98% Fe and P, accompanied by most of the critical impurities, including Al and Cu, were transferred into the solution. Then, a one-step spontaneous precipitation and phase transformation without acidity adjustment effectively synthesized battery-grade iron phosphate from the impurity-bearing acid solution. Surprisingly, it was noticed that there was an induction period for phase transformation from amorphous $\text{FePO}_4 \cdot x\text{H}_2\text{O}$ to monoclinic $\text{FePO}_4 \cdot 2\text{H}_2\text{O}$ during the precipitation. The critical crystal size for transformation was increasing along with the temperature, which was ascribed to the changes in the volume and surface energy. This research demonstrated the feasibility of chemically regenerating $\text{FePO}_4 \cdot 2\text{H}_2\text{O}$ precursors from the iron phosphate residue by precipitation purification in an acidic medium.

Biography:

Shili Zheng, Ph. D., is a professor at the Institute of Process Engineering, Chinese Academy of Sciences. He is currently the vice director of the National Engineering Research Center of Green Recycling for Strategic Metal Resources, China. He also serves as a member of the editorial board of the international journal of Hydrometallurgy. His research interests include the research and application of cleaner technology and secondary resource recycling, mainly focusing on the fundamental research and application development for efficient and cleaner extraction of metal resources, including vanadium, titanium, chromium, and lithium.

Sustainable Process for Mine Waste Utilisation and Critical Metals Recovery

Hong Peng^{1*}, James Vaughan¹, Penghui Yan¹, Tseveenkhuu Darinchuluun¹

¹*School of Chemical Engineering, The University of Queensland, Brisbane, Australia, 4074*

Abstract:

Extractive Hydrometallurgy has the long history to contribute the Australia economy in mining and mineral section. Following on the Australia Government's Critical Minerals Strategy 2023-2030, it is essential to build up advance sustainable extractive process by recovering valuable materials from waste and extracting critical minerals using innovative hydrometallurgical techniques. This talk will cover some research highlights on utilisation of mine tailings and urban mining waste for critical metals recovery and synthesis of value-added products (zeolites) for carbon capture and utilisation. The research is significant in addressing resource scarcity and environmental concerns while supporting the industries that depend on these essential materials.

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Biography:

Dr. Hong (Marco) Peng is now an Amplify Senior Lecturer at School of Chemical Engineering, the University of Queensland (UQ). He gained his PhD degree in Chemical Engineering at UQ with OZ Minerals Award for Excellent Thesis (2014). His research focuses on fundamental aspects of chemical engineering processes, with a specialization in unlocking nucleation and crystallization phenomena with projects on utilization of waste resource as functional materials for critical metals and carbon capture & utilization. Dr. Peng was the recipient of the prestigious Advance Queensland Industry Research Fellowships (Early & Middle Career) and UQ Amplify Fellowship.

Invited Talks

Research Progress on Clean and Efficient Recovery and Directly-Optimized Regeneration of Spent Lithium-Ion Battery Electrode Materials

Jianwen Liu*, Shiquan Wang, Xue Liu, Shaoqiang Liu, Junhan Pu

College of Chemistry and Chemical Engineering, Hubei University, Wuhan, China

Abstract:

In recent years, the recycling and re-utilization of spent lithium-ion battery electrode materials have gradually received widespread attention, and the reuse of spent cathodes and spent graphite anodes can effectively alleviate the resource tension, build a stable new energy industry supply chain, and achieve the long-term goal of carbon neutrality. Currently, the main recycling methods of spent lithium materials are pyrometallurgy and hydrometallurgy, which have high energy consumption and serious environmental pollution. To solve the above problems, our team achieved selective recovery of spent layered oxide material (NCM622) by deep eutectic salts, direct regeneration of NCM523 material by organic eutectic salts, and direct doping optimization of spent graphite by deep eutectic salts. These above works have realized the clean and efficient recycling and directly-optimized regeneration of spent lithium battery electrode materials.

Biography:

Dr. Jianwen Liu, professor, institute director, provincial innovation and entrepreneurship talent. The main research are focused on key materials for lithium/sodium/potassium ion batteries, nanomaterials electrochemistry, recycling of spent electronic products, etc. Until now, he has published more than 100 academic papers, authorized more than 20 invention patents. As the first completed person, he has won Hubei Science and Technology Progress Award, Hubei Economic Integration Award, and the Bronze Prize of National Post-doctoral Innovation and Entrepreneurship Competition. The main advanced scientific research achievements were reported in China News Network, Hubei Daily, Changjiang Daily, Hubei TV Station, and other medias.

Hydrothermal Treatment of Secondary Wastes from End-Of-Life Tire Pyrolysis

Tak H Kim^{1*}, Alexander Kelly², Austin Whittaker², Nicholas J Garozzo¹, Christopher L Brown¹

¹*School of Environment and Science, Griffith University, Nathan QLD 4111 Australia.*

²*Raw Power Systems Pty, Ltd, Southport QLD 4215 Australia*

Abstract:

The reduced carbon black underwent additional hydrothermal treatment and calcination to enhance its adsorptive capacity and broaden its potential applications. At each stage of processing, changes in the tire char were evident, including a reduction in mass. Subsequent investigation using inductively coupled plasma optical emission analysis (ICP-OES) revealed alterations in the overall composition of heavy metals, while X-ray photoelectron spectroscopy indicated shifts in surface elemental composition and bonding characteristics. The total heavy metal analysis indicated that concentrations of lead, cadmium, mercury, arsenic, and zinc in the processed material fell below the guidelines set by the international biochar initiative. Surface analysis revealed morphological changes during activation, with noticeable shifts in elemental composition and an increase in π - π interactions as activation progressed. To evaluate the adsorptive capacity, the activated tire char was tested against methylene blue, copper (II), lead (II), mercury (II), and cadmium (II). The maximum adsorption capacities demonstrated a significant increase at each stage of the activation process for most tests. When compared to a reference activated carbon, the calcined tire char exhibited markedly superior adsorption capabilities.

Biography:

Dr. Tak H. Kim is a lecturer in the School of Environment and Science and also serves as an Advance Queensland Industry Research Fellow at Griffith University, Australia. Since the completion of his PhD in nanocarbon materials in 2016, he has dedicated his effort to collaborating with small and medium-sized enterprises, working towards the development of practical solutions tailored to their specific needs. His research is centered on extracting valuable resources from disposed materials using sustainable processing techniques.

Session: Materials Chemistry

Keynote Talks

Assembly of Organic-Inorganic Hybrid Nanoparticles for Precision Nanobiotechnology

Zi (Sophia) Gu*

School of Chemical Engineering, University of New South Wales, Sydney, NSW 2052, Australia

Abstract:

Nanomedicine has emerged as a promising approach for precision treatment of life-threatening diseases such as cancers.¹ Nanomaterial innovation play a key role in driving progress of the field.² Organic-inorganic coordination nanoparticle-based therapeutic agents have been developed for safe and efficient cancer therapy.^{3,4} In this talk, I will present our recent work on developing programmable and precision cancer therapy by using copolymer-layered double hydroxide hybrid nanosheets and metal-organic framework. The nanoparticles were constructed via coordination chemistry, and demonstrated sensitive pH responsibility, biodegradability, tunable structure, and biomedical functionalities to deliver therapeutic and diagnostic payloads for targeted delivery, theranostics, drug repurposing, and catalytic nanomedicine.⁵⁻⁸

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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 pharmaceuticals and health. To date, she has published over 80 journal papers in the areas of nanomaterials and nanomedicine. She is an editor of *Journal of Nanobiotechnology and Exploration*, and an editorial advisory board member of *Small*.

Fabrication and Characterization of Two-Dimensional Inorganic/ Organic Materials and the Heterostructures

Minghu Pan^{1,2*}

¹*School of Physics and Information Technology, Shaanxi Normal University, Xi'an 710119, China*

²*School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China*

Abstract:

Research on two-dimensional (2D) materials and the heterostructures has been explosively increasing in last decade, stimulating the interests from condensed matter physics, electronic engineering, materials science, and chemistry. The unique structures and properties of 2D materials make them one class of the most appealing candidates for a wide range of potential applications. In particular, we have made some major breakthroughs in the field of 2D materials in last five years not only in synthesizing of monolayer or few-layer materials by ultrahigh vacuum molecular beam epitaxy (MBE) and chemical vapor deposition (CVD), but also in investigating exotic electronic phenomena in these 2D materials, *i.e.* topological bands, 2D superconductivity and 2D ferromagnetism, *etc.* Meanwhile, high resolution scanning tunnelling microscopy and spectroscopy (STM/S) and density functional theory (DFT) calculation, allow us to investigate the structure, electronic bands and properties of these compelling materials at the atomic scale and momentum space. Main findings, *i.e.* enhanced superconductivity in monolayer FeSe/SrTiO₃ heterostructure, topological flat bands in 2D hydrogen-bond organic frameworks (HOFs), chirality transferring in 2D assemblies of glycylglycine, ferromagnetism with record-high T_c in 2D Cr₅Te₈/CrTe₂ vertical heterojunctions, are summarized. Our works enrich the family of 2D materials and pave the

way to future innovative applications like electronics, spintronics and energy storage, etc.

Biography:

Minghu Pan is a Professor of Physics in Shaanxi Normal University and an adjunct professor of Physics at Huazhong University of Science and Technology. He received his PhD in condensed matter physics from Nanjing University in 2001. His research interests lie in experimentally studying the lattice, charge and spin on solid surface and low-dimensional materials using the powerful capabilities of the state-of-the-art scanning tunneling microscopy from the atomic scale to mesoscale, and the properties of surface/interface and thin-film materials, with a recent focus on 2D topological, superconducting materials and surface-based molecular chemistry. He has published > 120 SCI papers in high-profile journals, *i.e. Nat. Commun., Adv. Mater., Nat. Sci. Rev., Sci. Adv., Nano Lett., ACS Nano, PNAS, Phys. Rev. Lett., etc.* He was elected as Fellow of the International Association of Advanced Materials (IAAM), FIAAM in 2022 and awarded the IAAM Scientist Medal in 2023.

Save Energy Consumed by Catalysts for Water Electrolysis

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Abstract:

Overpotential in water electrolysis refers to the extra potential that exceeds the theoretical potential of 1.23 V, which is caused by energy losses in the circuit, the energy barrier of charge transfer, and unfavourable mass transport. Transition metal compound nanoparticles are frequently used as low-cost catalysts for HER and OER to increase active and specific surface areas for good electron transfer and mass transport. However, because of their poor conductivity and low mass transport for agglomeration, nanosized transition metal compounds are challenged by poor inter- and intra-particle charge transfer, which induces an overpotential to consume >80% extra energy for water splitting. To tackle the circuit energy consumption, we developed an ion-bridging method to optimize the charge transfer behaviour between two phases of nanocomposite.[1-3] We also developed confined growth of hierarchical nanostructures to fabricate MoP catalysts for HER to improve the mass transport in water splitting,[4] and ion-induced architecture and MOF templated construction of heterostructural composites[5-8]

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Biography:

Wenxian Li is a Future Fellow in the University of New South Wales (UNSW). He was a professor at Shanghai University before he joined UNSW. He received the Australian Postdoctoral Fellowship (Industrial) supported by the Australian Research Council in 2012 and then received financial support from the Australian Renewable Energy Agency as a Postdoctoral Fellowship. He joined the University of Western Sydney as a lecturer in the Solar Energy Technologies Group in November 2012. His research focuses on the electron configuration modulation-induced performance optimization of functional materials for renewable energy utilization.

Multifunctional Catalysts for Sustainable Chemicals and Fuels Production

Adam F. Lee*

Centre for Catalysis and Clean Energy, Griffith University, Australia

Abstract:

The anthropogenic origin of climate change from combustible carbon, and desire to establish a global circular economy is driving the quest for new sustainable manufacturing processes.¹ Catalysis has a rich history of facilitating energy efficient, selective molecular transformations, and will play a pivotal role in overcoming the scientific and engineering barriers to sustainable and economically viable energy vectors and chemicals. This presentation describes challenges in the design of catalytic technologies for biofuels and platform chemicals synthesis. Advances in the rational design of nanoporous solid acid and base catalysts enable the fabrication of hierarchical porous architectures² in which different active sites are spatially compartmentalised, permitting biodiesel production from low grade oils which cannot be processed by current technologies. Synergies between nanoporous solid acids and metal nanoparticles also facilitate active and selective upgrading of phenolic components of pyrolysis bio-oils to hydrocarbon fuels, and precious metal thrifting.³ Active site compartmentalization and flow chemistry facilitates chemical cascades to produce valuable chemical intermediates, exemplified by the cascade synthesis of cyanoesters² and γ -valerolactone.⁴

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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 *Materials Today Chemistry*, and recipient of the 2011 McBain Medal and 2012 Beilby Medal and Prize. Adam has co-authored >300 publications (h-index 78, 23,619 cites) and is a co-investigator and Flagship Project co-lead on the recently funded ARC Centre of Excellence 'Green Electrochemical Transformation of Carbon Dioxide' GetCO2.

Poster Presentations

Cu and Mn Co-Incorporated NH₂-MIL-125 for Efficient Photocatalytic CO₂ Reduction

Wenhao Gu¹, Jingxian Feng¹, Lulu Qiao¹, Di Liu¹, and Hui Pan^{1,2*}

¹University of Macau, Macao SAR, China

Abstract:

In this study, a series of Cu and Mn co-incorporated NH₂-MIL-125(Ti) (NML) with different Cu²⁺/Ti⁴⁺ and Mn²⁺/Ti⁴⁺ molar ratios are prepared via a convenient method (*i.e.* 1%Mn, 5%Cu, 1M-5C--NML; 3%Mn, 3%Cu, 3M-3C--NML; 5%Mn, 1%Cu, 1C-5M--NML). Due to the co-incorporation, the charge separation has been facilitated, which is responsible for the improved photocatalytic CO₂ reduction performance. After the irradiation, HCOOH was produced as the major product and the optimum 1M-5C--NML has shown the highest HCOOH yield, which has been improved 3.94 times compared with the pure NML. Among the co-incorporated samples, the electron paramagnetic resonance (EPR) signal intensity has increased with the increasing of incorporated Cu content, demonstrating the increasing generation of oxygen vacancy. In addition, the broad dipolar EPR peak without the well-resolved hyperfine peaks has shown with the increasing of incorporated Mn content, illustrating the formation of short-range Mn-Mn interactions. It is widely acknowledged that the oxygen vacancy could serve as electron trap to enhance the charge separation, leading to the improved photocatalytic production. On the contrary, the short-range Mn-Mn interactions could lead to a concentration quenching effect, leading to the negative effect on the photocatalytic production.

Biography:

Wenhao Gu was born at Nanjing, the capital of Jiangsu Province, China. He obtained his PhD in Environmental Science and Engineering, in Nanjing University of Information Science & Technology, China. His area of research is photocatalysis.

Acknowledgements:

This work was supported by the Science and Technology Development Fund (FDCT) from Macau SAR (0081/2019/AMJ, 006/2022/ALC, and 0111/2022/A2) Multi-Year Research Grants (MYRG-GRG2023-00010-IAPME and MYRG2022-00026-IAPME) from Research & Development Office at University of Macau, and Shenzhen-Hong Kong-Macao Science and Technology Research Programme (Type C) (SGDX20210823103803017) from Shenzhen. The DFT calculations were performed at the High Performance Computing Cluster (HPCC) of the Information and Communication Technology Office (ICTO) at the University of Macau.

Electrodeposition-Manufactured Ternary Metal Hydroxide Achieves Efficient Alkaline Water Electrolysis under Simulated Industrial Conditions

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¹*Institute of Applied Physics and Materials Engineering, University of Macau, Macao SAR, 999078*

²*Department of Physics and Chemistry, Faculty of Science and Technology, University of Macau, Macao SAR, 999078*

Abstract:

To achieve the international target for carbon neutrality, it is urgently required to increase the market for green hydrogen through water splitting driven by renewable powers. Most of laboratories electrodes were difficult to be fabricated on large scale in industry or unsuitable in industrially working environment that shall result in the instability of catalyst. Here, we devise a simple and industrially feasible electrochemical strategy for the preparation of catalyst. A series of hydroxides ($\text{Fe}_{7.5}\text{Co}_{7.5}(\text{OH})_y@ \text{NFF}$, $\text{Fe}_5\text{Co}_5\text{Ni}_5(\text{OH})_y@ \text{NFF}$, $\text{Fe}_{2.5}\text{Co}_{2.5}\text{Ni}_{10}(\text{OH})_y@ \text{NFF}$, and $\text{Ni}_{15}(\text{OH})_y@ \text{NFF}$) using for electrocatalysts, were growth on Ni-Fe foam (NFF) by tuning the electrolyte concentration. Notably, $\text{Fe}_{2.5}\text{Co}_{2.5}\text{Ni}_{10}(\text{OH})_y@ \text{NFF}$ not only exhibits ultra-low overpotentials (175 mV for 10 mA cm⁻²), but also has the superior Tafel slope (23.5 mV dec⁻¹) which has surpassed many reported OER electrocatalysts. Furthermore, the catalyst exhibits excellent stability, whether at low or high current densities during the OER process. Additionally, it still performed well in overall water-splitting stability testing. More importantly, the voltage of $\text{Fe}_{2.5}\text{Co}_{2.5}\text{Ni}_{10}(\text{OH})_y@ \text{NFF}$ showed only a small increase despite a simulated industrial water electrolysis environment with high temperature (60 °C), strong alkali (6 M KOH) and high current density (500 mA cm⁻²) after 1,000 hours of continuous operation. Meanwhile, its stability remains excellent for industrial alkaline water electrolysis (AWE). It can operate stably for more than 65 hours at a high current of 8 A (500 mA cm⁻²) with only slight degradation, showing potential for practical production applications.

Acknowledgements:

This work was supported by the Science and Technology Development Fund (FDCT) from Macau SAR (0081/2019/AMJ, 006/2022/ALC, and 0111/2022/A2) Multi-Year Research Grants (MYRG-GRG2023-00010-IAPME and MYRG2022-00026-IAPME) from Research & Development Office at University of Macau, and Shenzhen-Hong Kong-Macao Science and Technology Research Programme (Type C) (SGDX20210823103803017) from Shenzhen.

Biography:

Liu Chunfa is a doctoral candidate at Institute of Applied Physics and Materials Engineering, University of Macau. He is mainly engaged in the application of multi-metallic materials in water electrolysis.

High-Valence Metal Sites Enable Lattice Oxygen Activation Boosting Water Oxidation

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¹*Institute of Applied Physics and Materials Engineering, University of Macau, Macao SAR, 999078, China*

²Department of Physics and Chemistry, Faculty of Science and Technology, University of Macau, Macao SAR, 999078, China

Abstract:

Oxygen evolution reaction (OER) is recognized as kinetic constraint in water splitting. The oxidation-driven reconstruction in situ generates the corresponding hydroxides as actual active species, transition metal sites with high valence states can accelerate the reaction kinetics, enabling highly intrinsic activity. Here, we perform a NiFeCeO_x catalyst by electrodeposition as a model catalyst to investigate the influence of introducing Ce and Fe for Ni sites to toward OER. Introducing Ce promotes the in-situ reconstruction of NiO, generating active species NiOOH, greatly decrease over potential. Formation of Ni³⁺ as trigger of water splitting, however, is suffering from sluggish kinetics, resulting in high energy consumption at large current density. Fe component enables the formation of Ni⁴⁺, driving holes into oxygen ligand to facilitate intramolecular oxygen coupling, triggering lattice oxygen activation as ultimate catalytic center with highly intrinsic activity. The developed NiFeCeO_x exhibits superior OER performance with the overpotential of 218 mV at 10 mA cm⁻² and 659 mV at 500 mA cm⁻², respectively (without IR correction). This study provide insight understanding of OER and present valuable design guidelines for development of efficient OER electrocatalysts.

Funding Support:

Science and Technology Development Fund (FDCT) from Macau SAR (0081/2019/AMJ, 006/2022/ALC, and 0111/2022/A2) Multi-Year Research Grants (MYRG-GRG2023-00010-IAPME and MYRG2022-00026-IAPME) from Research & Development Office at University of Macau, and Shenzhen-Hong Kong-Macao Science and Technology Research Programme (Type C) (SGDX20210823103803017) from Shenzhen. The DFT calculations were performed at the High Performance Computing Cluster (HPCC) of the Information and Communication Technology Office (ICTO) at the University of Macau.

Biography:

Yunnan university (Double First-class B) 2014.09-2018.06

Yunnan University (Double First-class B) 2018.09-2021.07

Yunnan University (Double First-class B) 2021.07-2023.04 Research Assistant (RA)

University of Macau 2023.04-2023.08 Research Assistant (RA)

University of Macau 2023.08-Now. PhD

His research areas mainly focus on microstructural design and energy conversion of transition metal compounds

Spin Evolution and Flip in Oxygen Reduction Reaction: A Theoretical Study of Cu(Ni)XP₂S₆ (X = In, Bi and Cr)

Haoyun Bai^{1*}, Hui Pan¹

¹University of Macau, China

Abstract:

The local spin state has attracted increasing attention for its critical role to improve the catalytic performance in catalysis. However, the mechanism behind it has not been clearly

understood so far. Here, we carry out a theoretical study systematically to reveal the spin effect on the catalytic performance of metal compound in oxygen reduction reaction (ORR) based on density-functional theory (DFT). We find that Ni-incorporated two-dimensional (2D) CuXP_2S_6 (CNXPS, X = In, Bi, and Cr) show excellent activity for ORR, which is highly related to the spin transport and flip. Our results demonstrate that: (1) the high spin (HS) state of Ni ion is beneficial to ORR because of strengthened Ni-O bond and reduced total Gibbs free energy of system, which dominate the potential determining step; (2) spin flip occurs during the formation of Ni-O bond and breaking of O-O bond; and (3) the charge transfer during ORR is spin-sensitive due to the formation of O-H bond. Our findings specifically illustrate the effects of magnetic moment and spin on the system energy and bond strength, and the evolution of the spin during ORR, which may provide insightful understanding on the mechanism of spin-related ORR and guidance for the design of novel ORR catalysts with high performance. We thank the support from Science and Technology Development Fund (FDCT) from Macau SAR (0081/2019/AMJ, 006/2022/ALC, and 0111/2022/A2), Multi-Year Research Grants (MYRG-GRG2023-00010-IAPME and MYRG2022-00026-IAPME) from Research & Development Office at University of Macau, and Shenzhen-Hong Kong-Macao Science and Technology Research Programme (Type C) (SGDX20210823103803017) from Shenzhen. H. Bai also thank the support of UM Macao PhD Scholarship.

Biography:

Haoyun Bai is a Ph.D. candidate under supervision of Prof. Hui Pan in Applied Physics and Materials Engineering in University of Macau. He got the bachelor's degree from University of Electronic Science and Technology of China in 2020. He mainly focuses on the materials simulation via First-Principles Approaches, including catalysis, nano/micro-electronic devices, and spintronics. He had published 6 SCI papers as first author.

Two-Dimensional Janus Perovskite Oxynitrides as Active Photocatalysts for Overall Water Splitting with Ferroelectric Modulation

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Abstract:

Two-dimensional (2D) Janus structure is promising for photocatalytic water splitting because its intrinsic built-in electric field can overpass the requirement on the band gap of photocatalysts. However, how to achieve overall water splitting spontaneously in one structure is still difficult. Here, we present a novel family of 2D Janus perovskite oxynitrides, BaXNO_2 (X = Ta, Nb, V), with large intrinsic built-in electric field based on first-principles calculations. Both 2D BaTaNO_2 and BaNbNO_2 exhibit remarkable activity for photocatalytic overall water splitting. For BaNbNO_2 , a lowest overpotential of 0.44 V for oxygen evolution reaction (OER) is realized. The Gibbs free energy of hydrogen adsorption (ΔG_{H}) is near zero (0.02 eV) for BaTaNO_2 in hydrogen evolution reaction (HER). Interestingly, 2D BaVNO_2 shows the in-plane ferroelectricity due to the displacement of V ions, which modulates the band structures, resulting in optimized band alignment and improved light absorption for photocatalysis. The photocatalytic performance can be further improved by constructing a

BaNbNO₂/BaVNO₂ heterostructure, which has an overpotential of 0.47 V for OER and ΔG_{H} of 0.16 eV for HER. Our theoretical investigation provides not only a guidance to design Janus photocatalyst for full water splitting, but also strategies to modulate the photocatalytic performance through the ferroelectricity.

Fabrication and Characterization of Ultrathin Copper Foils by Accumulative Pack Rolling Process

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Abstract:

Copper foils have been widely used in electronic industry owing to their advantages of excellent conductivity, chemical resistance and good balance of strength and flexibility. With ever increasing interests in the fields of mobile phone, wireless broadband network and flexible electronics, copper foils are often used for current collectors, printed wiring boards, printed circuit boards and flexible printed circuit boards. These applications always require excellent surface quality, low-cost and ease of manufacturing for the copper foils. Cold rolling and electrodeposition are two main processes for the fabrication of copper foils. However, the surface roughness of copper foils fabricated using these methods is a challenge and an extra roughening treatment is always required. In this study, we have proposed an accumulative pack rolling (APR) process to manufacturing ultrathin copper foils with greatly improved efficiency. A minimum thickness of 2.2 μm can be obtained after the APR process. The microstructure and surface morphologies evolutions during APR process, and the effect of rolling direction have been comprehensively investigated.

Biography:

Ning Nie. He is currently a PhD student at University of Wollongong (Australia) conducting research on advanced rolling of metallic materials.

Microstructure Control of 2D Metal Based (hydr)Oxides for Water Electrolysis

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²Instrumental Analysis Center Taiyuan University of Technology, Taiyuan 030024, P. R. China

Abstract:

Hydrogen production technology from electrocatalytic water splitting has been widely concerned by various countries due to its ecological friendly and sustainable. hydrogen evolution reaction (HER) and Oxygen evolution reaction (OER) are the key reactions of electrolyzed water. Nevertheless, the large reaction barrier and slow reaction kinetics processes seriously affect the efficiency of hydrogen production, which could be improved by catalysts (platinum/carbon, and ruthenium or iridium oxides). However, such precious metal materials are expensive and scarce, which greatly limit the development of catalysts. Therefore, it is essential to design and develop low/non precious metal catalysts to reduce the use of precious metals and improve the activity of key reactions. Among them, 2D non-

precious transition metal-based nanosheets exhibit the characteristics of high specific surface area, abundant chemical active sites, and adjustable physical and chemical properties. In this study, morphological engineering, defect engineering, and doping engineering strategies were adopted to regulate the electronic structures of 2D non-precious transition-metal based catalytic materials, so as to improve their electrochemical performances.

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- [4] Advanced Science, 2023, 10, 2305194.

Biography:

Dr. Yanhui Song is an experimentalist of Taiyuan University of Technology (TYUT). She received Ph.D. in materials science from TYUT, China in 2021. She was studied as a joint Ph.D. student in Queensland University of Technology (QUT), Australia from 2019-2020. Her major research interests include metal (hydr)oxide nanomaterials for electrocatalytic applications.

Dissolution Energy Engineering by Conjugated Adsorptive Additives for Stable Aqueous Zinc-Ions Batteries

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¹University of Macau Taipa, Macau SAR, China; ²City University of Hong Kong, Hong Kong SAR, China.

Abstract:

The commercialization of aqueous Zn-ion batteries (AZIBs) for power-grid energy storage systems is hindered by the safety concerns arising from the zinc dendrite growth. The primary approach in addressing this issue is to induce planar depositions. However, modulating the Zn dissolution process which directly reshapes surface morphology and reserves growth sites has long been overlooked. Herein, by utilizing ester compounds as an illustration, we reveal that engineering the dissolution energy barrier is a pivotal factor in promoting homogeneous zinc dissolution. Ester adsorbents effectively redistribute charge densities at the electrode-electrolyte interface due to the presence of zincophilic ester functional group and conductive π -conjugation structure. This effect eventually facilitates Zn dissolution across the surface, transforming the pitholed and defective dissolution morphology into a smooth and consistent form. Thus, enhanced cycling stability can be achieved in both half-cells and full-cells, offering an extensive lifespan of thousands of hours for the dissolution and deposition cycles. This work provides a principle for the selection of Zn dissolution improvers to suppress Zn metal dendrite growth by regulating Zn dissolution behavior.

Biography:

Currently enrolled as a PhD student at the University of Macau, Mr. Li's research interests primarily lie in the field of new energy storage systems with aqueous electrolytes, specifically focusing on Zn-ion batteries. Additionally, he is engaged in the exploration of novel materials for energy conversion systems, particularly in relation to HER and OER.

Industrial Fabricated Si-Based Photoanode for Efficient and Stable Photoelectrochemical Water Splitting

Shuyang Peng^{1*}, Di Liu¹, Zhiqin Ying², Keyu An¹, Chunfa Liu¹, Jinxian Feng¹, Haoyun Bai¹, Kin Ho Lo¹ and Hui Pan¹

¹University of Macau, Macao S. A. R., China.

²Ningbo Institute of Materials Technology and Engineering, CAS, China.

Abstract:

Solar energy harvesting is an effective and sustainable method to solve the thorniest problems in this century. Among all the conversion methods, solar to fuel conversion by photoelectrochemical (PEC) cell is one of the most attractive means to transfer solar energy into green and inexhaustible hydrogen energy, which shows promising prospects. However, the fabrication cost and final PEC performance of recent products are not suitable for the practical application in solar fuel production. Therefore, we prepared photoanodes based on industrial Si with an easy fabrication method to investigate the possibility for industrial application. In this work, the n-Indus-Si/Co_{-2mA^{-xs}} photoanodes fabricated by electrodeposition show the minimum onset potential of 1.17 V vs. RHE and the highest saturation current density of 35.9 mA·cm⁻² under 1 solar power density. And it can maintain the current density of ~26 mA·cm⁻² for near 100 h until sample dropped in weak alkaline solution (0.25 M K₂B₄O₇, pH = 9.5). At the same time, a homojunction n-p⁺-Si/Pt/Co photoanode also shows a promising development direction. Our findings may provide new strategies to approach the requirement of large-scale PEC water splitting by proper engineering on industrial Si-based photoanodes, which shall guide the further development of practical solar energy conversion. We thank the support from the Science and Technology Development Fund (FDCT) from Macau SAR (0081/2019/AMJ, 006/2022/ALC, and 0111/2022/A2), Multi-Year Research Grants (MYRG-GRG2023-00010-IAPME, MYRG2022-00026-IAPME) from Research & Development Office at University of Macau, and Shenzhen-Hong Kong-Macao Science and Technology Research Programme (Type C) (SGDX20210823103803017) from Shenzhen.

Biography:

Shuyang Peng, who's major is Electromechanical Engineering, and the research interests are photoelectrochemical energy conversion and hydrogen production.

Scalable and Degradable Bioplastic Films from Moringa Oleifera Gum as Packaging Material

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Abstract:

The present study reports the synthesis of green, economical, and environmentally friendly biodegradable bioplastic films using a tree gum, *Moringa oleifera* gum (MOG). Herein, a series of bioplastic films were prepared using MOG and polyvinyl alcohol via thermal treatment followed by a solution casting method by varying the amounts of plasticizer, glycerol and crosslinker, citric acid to test their influence on the physiochemical properties of the synthesized films. All the films were evaluated using several characterization techniques.

The properties such as moisture content, water sensitivity, gas barrier attributes, tensile strength, the shelf life of packed food, and biodegradability were also investigated.

The results showed that all the plasticized films with higher CA amounts showed appreciable %elongation without compromising tensile strength, good oxygen barrier properties (0.013–0.189 barrer), packing efficiency, and biodegradation. Moreover, variations in the physicochemical properties of the synthesized bioplastic films from hydrophilicity to hydrophobicity and rigidity to flexibility make them a suitable candidate for their usage in food packaging applications. Since all the films were synthesized using economical and environmentally safe materials, and in contrast to the reported bioplastic films showed better physicochemical and barrier properties, thus proving to be a potential alternative to the conventional plastics.

Biography:

Dr. Ranote is presently a Marie Scklodowska-Curie Postdoctoral Fellow under Horizon 2020 within Marie Scklodowska-Curie Actions (COFUND) at the Centre of Polymer and Carbon Materials of the Polish Academy of Sciences, Zabrze, Poland. Presently, she is working on the synthesis of biodegradable, cost-effective multifunctional bioplastics. Her area of interest is interdisciplinary. Her research mainly focuses on multi-faceted applications of multifunctional materials developed from biowaste that are technologically highly attractive value-added accomplishments in the direction of sustainable development by biowaste utilization, low cost of the developed materials and overall green aspects of the work carried out.

Layer Hall Effect in Two-Dimensional Materials

Yangyang Feng¹, Baibiao Huang¹, Yandong Ma¹ and Ying Dai^{1*}

¹*School of Physics, State Key Laboratory of Crystal Materials, Shandong University, People's Republic of China*

Abstract:

Hall effect is an important electronic transport phenomenon, which can lead to novel physics and efficient device applications. In recent years, with the rise of 2D materials, the field of Berry curvature correlated Hall effects has undergone rapid development and received extensive attention at both the fundamental and applied levels. As a new member of the Hall effect family, the layer-polarized anomalous Hall effect (LPAHE) is proposed in MnBi₂Te₄ thin films. Here we state LPAHE in Van der Waals bilayer lattices. Three mechanisms that realize intrinsic LPAHE in bilayer lattices with different physical characters are proposed and studied. The first is for the ferromagnetic semiconductor with a band edge large Berry curvature, and the validity demonstrated in a real material of bilayer MnBi₂Te₄. The second is for the ferromagnetic semiconductor with valleytronic Van der Waals bilayers, which can be demonstrated in a series of real valleytronic materials, including bilayer VSi₂P₄, VSi₂N₄, FeCl₂, RuBr₂ and VClBr. The third mechanism of intrinsic LPAHE is for the multiferroic 2D systems with the coexistence of ferromagnetism, ferroelectricity, and valleytronics, and can be verified in the multiferroic material of bilayer Co₂CF₂. All of the mechanisms of the LPAHE are realized and manipulated by sliding ferroelectricity without employing external electric fields, especially for the LPAHE in multiferroic can be also appear without sliding ferroelectricity.

Biography:

Dr. Ying Dai is now working as a professor at School of Physics in Shandong University, P.R. China. Her current research interests focus on the electronic structure and related properties of functional materials, including semiconductor photo(electro)catalytic, spintronics properties and new physics effects of novel materials by means of first-principles calculation. More than 500 papers published in Phys.Rev.Lett., Nat. Commun., Nano Lett., Adv. Funct. Mater. and so on. Her H-index is 100. She has been named Highly Cited Researchers from 2018 to 2023 by Clarivate Analytics.

Exploration and System Construction of New Materials System

Baibiao Huang*

Shandong University, Jinan, China, 250100

Abstract:

Facing increasingly severe energy and environmental problems, accelerating the construction of new energy systems and promoting green and low-carbon energy development is the key to achieving China's comprehensive green transformation and "dual carbon" goals in economic and social development. Photocatalysis refers to the conversion of solar energy into storable chemical energy under mild lighting conditions, which is of great significance for accelerating the development of new and renewable energy in China, achieving energy structure transformation, and achieving the "dual carbon" goal. As the key to optoelectronics, there are still significant challenges in exploring and constructing new material systems for photocatalysis. Starting from the exploration of new materials and system construction, we have designed and prepared several new types of photocatalytic material systems, and built a new fuel cell photocatalytic system, providing new ideas for exploring and designing new photocatalytic materials and improving photocatalytic activity.

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Solvent-Induced Deformation of Aramid Nanofibers for Ultrahigh-flux Nanofiltration Membranes

Yuxi Ma^{1*}, Lifeng Wang¹ and Weiwei Lei¹

¹Institute for Frontier Materials, Deakin University, Victoria 3220, Australia

Abstract:

Aramid nanofibers (ANFs) are considered promising organic nano building blocks due to their high mechanical strength and chemical stability. They show potential in creating

energy-efficient membranes for wastewater recovery. However, existing ANFs often have small diameters, resulting in a dense membrane structure and a tiny pore size distribution that limits membrane permeability. To address this issue, we introduced a progressive protonation process to deform ANFs with diameters in the hundred nanometer scale. This process involved adding DMF as a secondary deprotonation solvent to DMSO, creating a mild deformation environment. The deformed ANFs were then utilized to develop membranes with a larger pore size distribution and higher surface charge by adjusting dispersion concentration. Remarkably, the water flux of these membranes can reach up to 40 times higher than commercially available nanofiltration membranes. Additionally, the membranes demonstrated high stability across a wide range of pH values and a 120-hour long-term testing period. These findings highlight the potential use of deformed ANFs for fabricating nanofiltration membranes as an efficient option for wastewater recovery. Furthermore, beyond DMF, other aprotic organic solvents, such as acetone and butanone, which share a similar molecular structure, can also deform ANFs with various diameters. This demonstrates the potential for precisely tuning the diameter of ANFs from a few nanometers to hundreds of nanometers or even micrometers.

Biography:

Yuxi Ma received the B.S. degree in Light Chemical Engineering from Soochow University, Suzhou, China in 2014 and the M.S. degree of engineering from Deakin University, Geelong, Australia in 2021. He is currently working toward the Ph.D. degree under the supervision of Weiwei Lei on the Institute for Frontier Materials, Deakin University, Geelong, Australia. His research interests include exfoliation of 2D materials and aramid nanofibers, nanofiltration membranes, solar steam and osmotic generators.

ZIF-8 Derived Carbon Supported Non-Noble Metal Catalysts for Oxygen Reduction Reaction

Haixia Zhang*

Taiyuan University of Technology, China

Selective Photocatalytic Conversion of Alcohol to Aldehydes by Singlet Oxygen over Bi-Based Metal-Organic Frameworks

Xiaoyang Zhang*

Shandong University, Jinan, China, 250100

Abstract:

In recent years, the selective oxidation of organic matter by solar photocatalytic means has attracted extensive attention. This process provides a new idea for energy storage and chemical synthesis in the field of artificial photosynthesis. So far, most of the work in photocatalysis has been devoted to the separation of photogenerated electron-hole pairs, and the possibility of using excitons (i.e., electron-hole pairs) for photocatalytic processes has not received much attention. In this work, we investigated the effect of metal dots on the stimulus behavior of two bismuth-based metal-organic frameworks (MOFs). Organic ligands (TATB and BTC) show different emission characteristics than their Bi-based MOFs. Specifically, TATB and BTC exhibit strong fluorescence emission, while Bi-TATB and Bi-BTC exhibit strong phosphorescent emission, suggesting that Bi-TATB and Bi-BTC have higher

inter-system crossover efficiency due to the heavy atom effect of Bi. The enhanced triplet excitation emission of Bi-TATB and Bi-BTC is further confirmed by the detection of $^1\text{O}_2$, as $^1\text{O}_2$ is known to be formed due to the energy transfer of the triplet state of the photosensitizer to the ground state oxygen ($^3\text{O}_2$). Based on the above understanding, Bi-TATB and Bi-BTC were finally used for the highly selective photooxidation of benzyl alcohol to benzaldehyde. This work provides a new understanding of the photophysical properties of Bi-based MOFs, and provides an alternative idea for the design of selective photooxidation materials.

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Radical-Induced Polymerization Enables Ultrafast Molecular Sieving via 2D Robust Nanochannels

Yue You^{1*}, Weiwei Lei¹, Shuaifei Zhao¹ and Jingliang Li¹

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Abstract:

Graphene oxides (GO) membranes with two-dimensional (2D) nanochannel open new avenues for maintaining high selectivity. However, their low permeability and low mechanical strength significantly limits their applications under realistic conditions. In this study, via a thermally induced radical polymerization strategy, the d-spacings of GO membrane nanochannels were controllably tailored (0.799 ~1.410 nm). The water permeance was achieved to $218 \text{ L m}^{-2} \text{ h}^{-1} \text{ bar}^{-1}$ (13 times higher than that of the pristine GO membranes) and a high molecule separation performance (> 95% rejections to Rose Bengal molecules). Furthermore, even under realistic conditions (pH from 4.0-10.0, up to 12 bar and 40 °C), the water permeance stability was reached to $140 \text{ L m}^{-2} \text{ h}^{-1} \text{ bar}^{-1}$ in a long-term operation (200 h). Meanwhile, the hydrogen-bond frameworks introduced from N-Vinylformamide (NVF) chains led to a high mechanical performance. The swelling ratio of the nanochannels significantly reduced from 60.08% to 10.76% and the mechanical strength increased 210% (from 34 MPa to 105 MPa). This strategy for tailoring 2D nanochannel via radical polymerization in this work not only overcomes the trade-off between permeability and selectivity of the 2D membrane, but also presents a facile technique for engineering advanced performance 2D membranes with stable and adjustable nanochannels.

Biography:

Yue You is currently a Ph.D. candidate in Institute for Frontier Materials at Deakin University under the supervision of A/Prof. Jingliang Li, A/Prof. Weiwei Lei, and Dr. Shuaifei Zhao. She received her master's degree from Monash University in 2019. Her current research focuses on the development of nanostructured materials and membranes for water treatment.

ROOM A**Session: Materials for Energy Conversion and Storage****Keynote Talks****Red TiO₂: Color Origin and Present Status****Li-Chang Yin^{1*}, Kangyu Zhang¹, Gang Liu¹, and Hui-Ming Cheng²**¹*Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China.*²*Institute of Technology for Carbon Neutrality, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, 1068 Xueyuan Blvd, Shenzhen 518055, China.***Abstract:**

Introducing band-like doping levels, thus narrowing the bandgap of wide bandgap metal oxides is highly desirable for developing highly efficient photocatalysts with wide spectrum and strong absorption. Identifying the prerequisite of inducing band-like doping levels in wide bandgap metal oxides is a crucial yet open question. Herein, we took boron (B) and nitrogen (N) codoped anatase TiO₂ as a model system, and resolved this question by combining density functional theory (DFT) calculations with machine learning (ML) methods enabled by a newly designed structure descriptor. The results indicate that the band-like doping levels originate from the strong *p-d* coupling between O/N-*p_π* and Ti-*t_{2g}* orbitals. Significantly, the presence of strong *p-d* coupling is actually an intrinsic characteristic of anatase TiO₂, entirely determined by crystal symmetry rather than being restricted to specific doping configurations. Therefore, it is universally applicable for determining whether inducing band-like doping levels is feasible, and has been fully verified on six more metal oxides including rutile and brookite TiO₂, WO₃, SnO₂ as well as MgTa₂O₆. Besides, the strong *p-d* coupling offers a theoretical basis for the long-held experimental understanding that uniform doping is important for achieving better photocatalytic performances of metal oxides. Overall, the uncovered strong *p-d* coupling provides a simple yet profound guideline for bandgap engineering of metal oxides. At the end of this talk, the recent progress on the photocatalytic water splitting performance based on red TiO₂ will also be briefly introduced.

Biography:

Professor, Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences. Graduated (Ph.D) from Jilin University in 2002, focusing on the theory and simulation of advanced energy conversion materials. Published more than 160 peer review papers with the total citation over 18,000 times and the H-index of 56 (Google Scholar). Clarivate Highly Cited Researcher (2020-2023).

Materials Advances for Robust Proton Exchange Membrane Fuel Cells

Daniel HC Chua*

National University of Singapore, Dept of Materials Science & Engineering, 9 Engineering Drive 1, Singapore 117575

Abstract:

Proton exchange membrane fuel cells (PEMFC) are among the most promising clean power generators for tomorrow's energy needs as these are essentially power generators. It is well-known that low temperature PEMFC are highly suitable for mobile and transportation applications due to its low temperature operations and high efficiency. Furthermore, it has other advantages such as no moving parts, solid electrolyte, silent operations and emission of useful by-products, which is drinkable clean water. Currently, durability and reliability remain as the main key challenges today. We will show that advancement in carbon-backed materials can overcome the reliability issue. Through a series of design mix and match, we are able to form hybrid/composites which we can engineer into a fully integrated membrane electrode assembly. This has shown to have the desired properties required for PEM fuel cells operations. For example, we demonstrate that hybrid structures of 1D carbon materials have unique advantages over the standard carbon black (VXC-72R). We can further integrate 1D/2D hybrids where excellent energy conversion and robust properties have been obtained. In all the work done, a series of in-situ tests are also performed which includes accelerated degradation test, AC Voltammetry and electrochemical impedance spectroscopy and different charge/discharge test to validate the effectiveness and robustness of these materials.

Biography:

Associate Professor Daniel Chua joined the Department of Materials Science and Engineering at the National University of Singapore in 2005 where he started as a junior faculty. He was awarded the NUS Young Investigator Award in 2008. He received his Ph.D in Engineering in 2004 from University of Cambridge and prior, his BSc (Honours) from the National University of Singapore. He has several years of working experience in semiconductor and harddisk media where he worked as a failure analysis and materials engineer before joining as an academic. His current area of interest focusses on application of designing and developing nanostructured materials with applications in clean energy and environmental work.

Hydrogen-Rich B Containing Systems for Hydrogen Storage

Zhenguang Huang*

University of Technology Sydney, 81 Broadway, Ultimo, Sydney, NSW 2007

Abstract:

Hydrogen-rich B containing systems have been extensively studied as hydrogen storage materials. In this talk, I will present several systems. I will discuss reactions between amine-borane complexes and amines which generate high purity H₂ gas under ambient conditions. For example, the reaction between ethylenediamine bisborane (EDAB) and ethylenediamine (ED) leads to unique boron-carbon-nitrogen 5-membered rings in the dehydrogenation product where one boron is tri-coordinated by three nitrogen atoms. Due to the unique cyclic structure, the dehydrogenation product can be efficiently converted back to EDAB by NaBH₄ and H₂O at room temperature. I will then talk about the first synthesis and characterization

of 1,6;2,3-bis-BN cyclohexane, an isostere of cyclohexane with two adjacent BN pairs. Its ring flipping barrier is similar to that of cyclohexane. Protic hydrogens on N in 1,6;2,3-bis-BN cyclohexane show higher reactivity than its isomeric bis-BN cyclohexane. This compound exhibits an appealing hydrogen storage capability of >9.0 wt%, nearly twice as much as the 1,2;4,5-bis-BN cyclohexane. Our research demonstrates the potential of hydrogen-rich B containing systems as hydrogen storage materials.

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Synchrotron Radiation Study on MXene-Based Energy Materials

Li Song*

National Synchrotron Radiation Laboratory, School of Nuclear Science and Technology, University of Science and Technology of China, China

Abstract:

Due to their ultrathin layered structure and rich elemental variety, two-dimensional layered transition metalcarbides/nitrides (MXenes) are emerging as promising energy materials for energy generation and storage. In principle, MXenes can be produced by selective etching of the A-layers from their MAX phases, exhibiting a hexagonal crystal structure with transition metal carbide/nitride layers. Due to the involvement of both anions and cations in the etching reactions, it is still high challenge to obtain detailed information, such as phase evolution, lattice change, etching time scale, and so on. Therefore, it is highly desired to develop in-situ and operando techniques to further study realize the real-time monitoring of the complicated and fast etching process, as well as to better understand the real working mechanism of MXenes in energy storage and conversion applications. Here, we will present our resent results on MXene-based energy materials by means of various synchrotron radiation X-ray techniques and methods.

Biography:

Prof. Song received Ph.D. from Institute of Physics CAS in 2006, then worked at University of Munich Germany, Rice University USA and Shinshu University Japan. In 2012, he was promoted to professor at University of Science and Technology of China, leading a multi-technique research team in Hefei Light Source. His research focuses on the development and application of synchrotron radiation-based new technologies and methods for nanomaterials and nanodevices. So far, he has published about 400 scientific papers with over 42000 citations (H-index 100), continuously nominated as the global highly cited scientist by Clarivate in 2019-2023.

Rational Catalyst Design for CO₂ Electrochemical Reduction Reaction

Ziyun Wang*

School of Chemical Sciences, The University of Auckland, Auckland 1010, New Zealand

Abstract:

Selectivity is very important in the electrochemical reduction of CO₂ (CO₂RR), both scientifically and industrially. Recently, C₂ selectivity has exceeded 80% on Cu-based catalyst using the flow cell, and ethylene and ethanol are the main two products. Understanding the mechanism branching the ethylene and ethanol is the key to achieve high selectivity of CO₂RR.

In this work, we first used density functional theory (DFT) calculations to understand the reaction pathways of CO₂RR to ethylene and ethanol. The reaction barriers and enthalpy changes are calculated for the elementary steps considered in the two pathways on Cu(100). Based on the DFT results, we investigated two factors that could affect the ratio between ethylene and ethanol, namely CO coverage and surface decoration. Using DFT calculation, we found that CO coverage could affect the relative energies of intermediates along ethylene and ethanol pathways, thus favoring one product over the other. With the decrease of CO coverage, the ethylene pathway becomes more favorable. Experiment results suggest the same trend and the highest ethylene selectivity is achieved with low CO partial pressure in CORR experiment. We also investigated the effect of surface decoration and found metal oxide and surface condiment favors ethanol.

Biography:

Dr. Ziyun Wang is a computational chemist specializing in theoretical catalysis and machine learning. He conducted his doctoral research in theoretical catalysis at the Queen's University of Belfast under the guidance of Prof. Peijun Hu and Prof. Chris Hardacre. This was followed by postdoctoral research with Prof. Jens Nørskov and Prof. Thomas Bligaard at Stanford University, and with Prof. Edward Sargent at the University of Toronto. In 2021, Dr. Wang joined the School of Chemical Sciences at the University of Auckland, where he is currently a Senior Lecturer.

Advanced Electrode and Electrolyte Materials for Potassium Ion Batteries

Jianfeng Mao*

Presenter and Co-author names {For Ex: (David Mansom^{1*}, John Smith¹, Fred Cox¹)}*

School of Chemical Engineering, The University of Adelaide, Adelaide, SA, 5005 Australia

Abstract:

The development of advanced energy storage systems is urgent to transform our society into one based on renewable energy resources, in which rechargeable batteries are one of the most promising approaches but remains to be solved. Aqueous Zn metal batteries promise high capacity, low cost, high safety, and sustainability for large scale energy storage. Their Zn metal anode suffers, however, from side reactions and dendrite growth that occur at the Zn-electrolyte interface, and these considerations limit their full potential. Regulating the electrolyte formulation for in-situ construction of highly Zn²⁺-conductive solid-electrolyte interphase is a promising approach to handling these interface-related issues. In this talk, I will introduce our recent work on rational electrolyte design and interphase engineering for Zn metal batteries [1-4] and will discuss the issues and opportunities for building better batteries.

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Biography:

Dr Jianfeng Mao is a Senior Lecturer, ARC Future Fellow and the inaugural Discipline Lead in Materials Engineering at the School of Chemical Engineering, the University of Adelaide. His current research interests are in developing functional materials and electrolytes for next-generation batteries, and understanding their fundamentals of electrochemical processes in electrodes and at electrode/electrolyte interfaces. He has published over 100 papers (60+ as the first or corresponding author) in the leading discipline journals, such as *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*, *Adv. Mater.*, *Energy Environ. Sci.*, *Nat. Commun.*, *Sci. Adv.*, and so on. These publications have received over 9,600 citations, giving an h index of 49 at Google Scholar (December 2023).

Invited Talks

Electronic State Modulation in Semiconductor Materials towards Photocatalytic CO₂ Reduction Performance

Hefeng Cheng*

Shandong University, China

Abstract:

The electronic structure of semiconductor materials, i.e., the electronic state, is the key factor that determines the photocatalytic performance of semiconductor materials. Hence, rationally design of efficient photocatalysis depends on the effective modulation of the electronic state. As artificial photosynthesis that enables to reduce CO₂ to high value-added hydrocarbon fuels, is regarded to be a promising strategy to alleviate the energy crisis and achieve carbon neutrality. However, CO₂ molecules are difficult to activate, and CO₂ reduction is a multi-electron-proton coupling process, involving a variety of intermediates, resulting in unsatisfied activity and selectivity of the products.

Recently, we have improved the activity and selectivity of photocatalytic CO₂ reduction performance by manipulating the electronic state of semiconductor materials through precise defect designs. In an earlier work, we anchored the Au single atom to the surface of the ZnIn₂S₄ nanosheet by the ligand exchange strategy, which achieved high activity and high selectivity for photocatalytic CO₂ reduction to CH₄. In situ infrared spectroscopy combined with theoretical calculations showed that the Au₁/ZnIn₂S₄ catalyst with low coordination structure could effectively activate CO₂ molecules, stabilize *CO intermediates, and further protonation to CH₄.

Biography:

Dr. Hefeng Cheng is now a professor at Shandong University. He obtained the Ph.D. degree

in 2012. His main research interest covers semiconductor defect chemistry, photo(electrical) catalysis, surface plasmon catalysis and other solar energy utilization and conversion. He has published more than 30 papers in journals such as JACS and Angew. Chem as the first or corresponding author. With an H-index of 43, his total number of citations of the papers has exceeded 7,000 times, and six of them have been selected as ESI Highly Cited Papers.

High Entropy Alloy Enables Efficient CO₂ Redox Reactions

Shilin Zhang^{1*}, Liang Sun¹ and Zaiping Guo¹

¹*School of Chemical Engineering, The University of Adelaide*

Abstract:

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

Biography:

Dr Shilin Zhang is now a research fellow at the University of Adelaide, Adelaide, Australia. He received his PhD degree from the Institute of Superconducting & Electronic Materials in the University of Wollongong (Australia) in 2020 under the supervision of Prof. Zaiping Guo, after he graduated from Beijing University of Chemical Technology with an MSc in 2016. His current research interests focus on the design, synthesis and characterisation of electrode/electrolyte materials in the field of batteries.

Physics and Design of Two-Dimensional Semiconductors and Heterostructures for Sustainable Nanoelectronics Applications

Yee Sin Ang^{1*}, Chuin Wei Tan², Che Chen Tho¹, Xukun Feng¹, Qianqian Wang¹ and Liemao Cao³

¹*Singapore University of Science and Technology (SUTD), Singapore;*

²*Harvard University, USA;*

³*Hengyang Normal University, China*

Abstract:

We introduce and review the recent advances on the computational design and modelling of two-dimensional (2D) semiconductor and heterostructures. We show that the emerging monolayer family of MA₂Z₄ exhibits strong potential in electronics, optoelectronics, and deep ultraviolet (UV) applications. The design of Ohmic contacts to MA₂Z₄ 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. 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. These results shall provide a step forward towards the development of a more sustainable computing electronics landscape beyond the conventional silicon device technology.

Biography:

Dr. Yee Sin ANG is an Assistant Professor at the Singapore University of Technology and Design (SUTD). His research focuses on the use-inspired basic research of low-dimensional and topological materials (theory and simulation). His current research topics include charge injection physics of 2D materials (e.g. thermionic, field and photoemission), quantum transport phenomena (e.g. nonreciprocal and non-Hermitian effects), computational design of sub-10-nm transistor, and *beyond CMOS* computing architecture such as reversible computing, valleytronic and neuromorphic devices. Dr. Ang is listed in the World's Top 2% Scientists (Applied Physics) by Stanford University/Elsevier in 2022 and 2023, and in the Emerging Leaders of *Journal of Physics D: Applied Physics* (Class of 2022). Dr. Ang is also an alumni of the 59th Lindau Nobel Laureate Meeting (2019).

Halide Perovskite for Photocatalytic H₂ Evolution

Peng Wang^{1*}, Qianqian Zhang¹ and Baibiao Huang¹

¹State Key Laboratory of Crystal Materials, Shandong University, Jinan, China

Abstract:

Hydrogen iodide (HI) splitting is a promising way to produce H₂, which is conventionally investigated in thermochemical industry area in the iodine–sulfur cycle, and has caught increasing attention in halide perovskite photocatalysis.[1] The innovative system was first established in hydroiodic acid saturated with MAPbI₃, where existed a dynamic equilibrium between the perovskite solute and saturated solution, maintaining the long-term stability of MAPbI₃ microcrystals in aqueous HI solution. In terms of a rising photocatalytic system, it is of great significance to explore the modification methods to enhance the photocatalysis efficiency feasible in the special catalytic conditions. From the viewpoint of improving the utilization efficiency of photogenerated carriers, methods corresponding to surface modification and composition adjustment are applied to promote carrier transfer and charge separation respectively. Specifically, i) MAPbI₃/rGO composite was fabricated through a facile photoreduction method, obtaining a 67 times higher photocatalytic H₂ evolution reaction (HER) rate than that of the pristine MAPbI₃. The H₂ evolution from H⁺ proceeded at the rGO sites by rapid extraction and transportation of photogenerated electrons from MAPbI₃ via Pb–O–C linkages.[2] ii) Mixed-halide perovskite MAPbBr_{3-x}I_x was exploited in mixed HI/HBr solution through the ion exchange method, which possessed an iodide concentration gradient distribution to form a bandgap funnel structure for charge-transfer. The HER activity was substantially enhanced and a STH of 1.05% was obtained.[3] iii) It was also found that the halide ion concentration gradient was also viable in all-inorganic perovskite, and

CsPbBr_{3-x}I_x with a graded band alignment was prepared, showing an elevated photocatalytic HER activity.[4].

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Biography:

Peng Wang got Ph.D from Shandong University in 2010, then did posdoc research in Prof Domen's group in Tokyo Univeristy, then did research in Argonne National Lab. In 2015, he joined Shandong Unviversity in 2015. His research is focused on Plasmonic photocatalyst, PEC, HER, and perovskite for HER.

The Research Progress of High Bandgap Cu₂ZnSnS₄ Solar Cells

Kaiwen Sun^{1*}, Jialiang Huang¹, Ao Wang¹, Xiaojie Yuan¹, Xin Cui¹, Martin Green¹ and Xiaojing Hao¹

¹*School of Photovoltaic and Renewable Energy Engineering, University of New South Wales, Sydney, NSW, 2052, Australia*

Abstract:

High bandgap sulfide kesterite Cu₂ZnSnS₄ (CZTS) provides an attractive low-cost, environmentally benign and stable photovoltaic material, and represents a promising top cell candidate for thin film/Si tandem solar cell technology. University of New South Wales (UNSW) has been working on high bandgap CZTS since 2013, aiming to develop high efficiency, cost-effective thin film top cell for applications in Si based tandem. This presentation will summarize the research progress of the high bandgap CZTS at UNSW, discussing the key strategies and milestones for achieving efficiency breakthrough during the R&D process. The kesterite absorber^{1,2}, front heterojunction interface³⁻⁵ and kesterite/back contact interface⁶ are the three main regions have been focused. The future development direction and insight will also be touched.

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Catalysts Design Promoting N² Electrofixation

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Key Laboratory for Soft Chemistry and Functional Materials, Nanjing University of Science and Technology, Ministry of Education, Nanjing, 210094, China

Abstract:

It has been long believed that FeMoS structure, where Fe is bonded with S, plays a pivotal role as a biomimetic catalyst for electrochemical nitrogen (N₂) fixation. Nevertheless, the structure of Fe bonded to heavier analogues (Se or Te) has never been explored for N₂ electrofixation. Here, we theoretically predict the electronic structure of FeMo(Se, Te) composed of tri-coordinated Fe species with open shells for binding with Se, which forms a collective electron pool for promoting N₂ activation. Guided by this interesting prediction, we then demonstrate a two-step procedure to synthesize such structures, which displays remarkable N₂ electrofixation activities with ammonia yield of 72.54 μg h⁻¹ mg⁻¹ and Faradic efficiency of 51.67% that are more than three times of the FeMoS counterpart. Further mechanism study has been conducted through density function theory (DFT) simulations. This work would provide new clues for designing versatile electrocatalytic materials for large-scale industrialization

Biography:

Professor Sheng CHEN has devoted to the design, preparation and application of low-dimensional nanomaterials for carbon-neutral energy catalysis. He has served as the academic editor, editorial board member and young editorial board member for such journals as *Exploration*, *Catalyst*, *Carbon Energy*, *Journal of Energy Chemistry*, *Carbon Neutralization*, etc. He is also the Member of the Expert Committee of Chinese Energy Society. Within the past years, he has studied and worked at Nanjing University of Science and Technology (PhD), Monash University (exchange student), University of Adelaide (Postdoctoral), University of New South Wales (Research fellow) in Australia and Max Planck Institute of Colloids and Interfaces in Germany (Alexander von Humboldt Fellowship). He has published more than 100 papers in world-leading journals like *Nature Communications*, *Angew Chem Int Ed*, *Advanced Materials*, *ACS Nano*, *Energy Environmental Science*, etc. His research papers have received more than 13,000 citations. Further, he has been awarded as world's top 2% most-cited scientists, ESI Highly Cited Researcher (Clarivate), China's Highly Cited Scientists (Elsevier), and international association for advanced materials (IAAM) scientist award. He has filed/applied more than 20 invention patents and developed new materials/techniques that have been widely industrialized.

Controlled Growth and Electrocatalytic Hydrogen Evolution Property Tuning of TMDCs

Peizhi Liu^{1*}, Bing Hao¹, Dechuan Peng¹, Jingjing Guo¹ and Junjie Guo¹

¹Key Laboratory of Interface Science and Engineering in Advanced Materials, Ministry of Education, Taiyuan University of Technology, China

Abstract:

Transition metal dichalcogenides (TMDCs) are an attractive novel 2D materials with high possibilities of replacing noble metal-based catalysts in hydrogen evolution reaction (HER). Molybdenum disulfide (MoS_2) and platinum diselenide (PtSe_2) nanosheets were synthesized and exhibited comparable HER electrocatalytic properties with commercial Pt/C catalysts. To enhance the electrocatalytic hydrogen evolution properties of PtSe_2 based catalysts further, and reduce the consumptions of noble metals at the same time, non-noble metal doping and heterointerface engineering were adopted. Pt, PtCo and PtCu nanosheets with controlled crystallographic orientation were prepared as precursors by a hydrothermal process, and the following insufficient selenization in a tube furnace produced high-efficiency HER electrocatalysts constructed with PtCo/ PtSe_2 and PtCu/ PtSe_2 heterojunctions. The catalysts exhibit a low overpotential of 38 mV and 47 mV at a current density of 10 mA cm^{-2} , a small Tafel slope of 22 mV/Dec and 44 mV/Dec respectively, and a superior stability in a standard HER test with a sulfuric acid solution of 0.5 M. It is demonstrated that the electrocatalytic active sites can be tuned with crystal facets of TMDCs nanosheets, and the improved activity of the catalysts arises from a synergistic effect of the heteroatom doping and heterojunctions. The newly developed TMDCs catalysts can provide new ideas for the design of highly efficient HER electrocatalysts, and will promote the development of green hydrogen energy industry.

Biography:

Dr. Peizhi Liu is an associate professor in the Key Laboratory of Interface Science and Engineering in Advanced Materials, Ministry of Education, at the Taiyuan University of Technology, and his research focuses on electron microscopy, material interfaces, and 2D materials. He received his bachelor of engineering with the major of Materials Science and Engineering from Central South University in 2009, and PhD in Materials Science in 2014 from the University of Tennessee. He has authored or co-authored more than 50 technical papers and has contributed several technical presentations at national and international conferences.

Nonmetallic Plasmonic Materials for Photocatalysis

Zaizhu Lou*

Jinan University, Guangzhou, 510632, China

Abstract:

Surface plasmon resonance (SPR) is unique optical properties of noble metal nanoparticles (NPs), which have been applied in various fields including biological molecular sensor, photo-detection, and photoenergy conversion. Recently, plasmonic metal NPs have attracted attentions for photocatalysis attributing to their strong visible light absorption in solar energy harvesting. However, the rarity and high-cost of noble metals NPs limited their large-scale application in photocatalysis. The low-cost nonmetallic plasmonic materials with broad light response have been the ideal substitutes of plasmonic metals for photocatalysis. In recent years, our research group focused on the synthesis of nonmetallic plasmonic photocatalysts, their applications and mechanisms in photocatalysis. Several efficient strategies including "photoelectron injection" and "electron accumulation" were developed by constructing nonmetallic plasmonic heterostructures, which improved the electron density of plasmonic materials leading to enhanced photocatalysis for CO_2 reduction and hydrogen generation. To quantify the detailed contributions of photoelectron, hot electrons and photothermal

effect of nonmetallic plasmonic photocatalysts in enhancing catalysis, we demonstrated the dominant role of hot electron on boosting photocatalysis by reducing reaction barriers, and high-efficient nonmetallic plasmonic heterostructures $W_{18}O_{49}$ -rGO were developed as photocatalysis for alcohol dehydration reaction.

Biography:

Dr. Zaizhu Lou obtained the Ph.D. degree in 2014 at Shandong University, and joined Osaka University as JSPS Research Fellow in 2015. Now, he is Full Professor of Jinan University. He has published over 70 SCI-indexed papers on Nat. Commun., Proc. Natl. Acad. Sci. U.S.A., Adv. Funct. Mater., ACS Nano, Appl. Catal. B-Environ. et al. He was awarded as JMCA Emerging Investigator, Vebleo Fellow, and Distinguished Young Scholars and Young Pearl River Scholar from the Guangdong Government. His research interests are in the field of plasmonic photocatalysis.

Optimising The Flow Behaviours in Flow Channels *via* CFD Modelling to Accelerate Electrolyser Performance

Yuting Zhuo^{1*} and Yansong Shen¹

¹*School of Chemical Engineering, University of New South Wales, Sydney, NSW 2052*

Abstract:

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

Biography:

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

Nanomaterial and Coating for Solar Energy Applications and Perovskite Solar Cells

Dr. Pisist Kumnorkaew*

National Nanotechnology Center (NANOTEC), Thailand

Abstract:

The innovative nanocoating research team at NANOTEC Thailand focuses on the development of solution-based nano coatings for industrial applications, particularly in solar energy. These applications include solar thermal systems, commercial solar cells, and emerging solar cell devices. In solar thermal applications, a low-cost solar absorber coating made of graphene/nano silica has been developed to enhance the conversion of solar radiation into heat. This coating has enabled the generation of superheated steam at 450°C and 30 bar pressure. It has been used in parabolic trough and linear Fresnel solar concentrators in various factories. For commercial solar cells, a transparent, anti-dust nanocoating made from surface-modified nano silica has been developed to maintain electricity production and reduce maintenance costs in solar farms and on solar roofs. This coating solution is designed for easy, on-site application.

For emerging solar cells, semiconductor nanomaterials such as tin oxide, titanium dioxide, and zinc cadmium sulfide have been developed as electron-transporting materials to enhance the performance and stability of perovskite solar cells, which are expected to be the next generation of solar cells. The NANOTEC team achieved a power conversion efficiency of over 21.4% and a stability of more than 2400 hours without encapsulation. Additionally, perovskite modules with open circuit voltages of 7V and 12V were fabricated on 5x5 and 10x10 sq. cm substrates, respectively.

Silicon-Based Anode Materials for Energy Storage Systems

Lei Zhang*

Centre for Catalysis and Clean Energy (CCCE), Griffith University

Abstract:

Si-based materials have garnered extensive attention as anodes for lithium-ion batteries (LIBs), with their cycling stability hindered by significant volume expansion during lithiation. An effective strategy to address this challenge involves creating void space within the material structure, exemplified by yolk-shelled Si/C structures, which have shown remarkable improvements in LIB cycling performance.

However, traditional yolk-shell structures face limitations due to complex and environmentally unfriendly fabrication processes, impeding their widespread application. Moreover, inherent structural defects in traditional yolk-shell designs have been identified. In this presentation, we will introduce novel, scalable fabrication methods aimed at overcoming the challenges associated with preparing yolk-shell electrode materials. Additionally, we will present a next-generation yolk-shell Si/C anode material that fundamentally addresses electrochemical deficiencies, offering a promising solution for advanced LIB technology.

Biography:

Dr. Lei Zhang, with a Ph.D. in Material Science from the University of Wollongong, is currently a DECRA Fellow at Griffith University. His research focuses on the application of high-energy-density electrode materials in battery systems and the utilization of novel in-situ detection technologies for battery characterization and failure analysis.

MXene-Based Membranes for Clean Energy Harvesting

Guoliang Yang^{1*}, Yozelin Zavala-Galindo¹, Si Qin¹, Yuxi Ma¹, Lifeng Wang¹, Zhiyu Wang¹, Weiwei Lei¹ and Dan Liu¹

¹Institute for Frontier Materials (IFM), Deakin University, Australia

Abstract:

Utilizing the salinity gradient between river water and seawater has been an attractive, renewable, and clean way to generate energy, so-called 'blue energy'. Another electrokinetic phenomenon, called the streaming potential, occurs when an electrolyte is driven through a charged material either by a pressure gradient¹ or by an osmotic potential deriving from a salinity gradient². Currently, several methods have been conducted to harvest the above clean energy, majority of which are founded on separation system by utilizing membranes³. MXenes, a new family of 2D nanomaterials, were firstly found and synthesized from their parents, MAX phase, in 2011. Because of their special structures, MXenes have been investigated to possess excellent electric, thermal, mechanical, and optical properties. More importantly, the abundant surface groups, like -F, -O and -OH, make the MXenes with superior hydrophilicity, which is significant for fabricating 2D laminate membranes. Meanwhile, the zeta potential of the $Ti_3C_2T_x$ was measured to be -34.75 ~ -63.3 mV,^{4, 5} which could form considerable surface charge density of the MXene-based membranes. Based on these excellent properties, we designed layered pristine MXene membranes and MXene-based nanocomposite membranes with various structures such as polyelectrolyte functionalized 2D nanochannels, mixed 2D/2D nanochannels, 2D/2D Janus structure, for clean energy harvesting, including electrokinetic energy conversion and osmotic energy harvesting. MXene-based membranes are shown to be promising candidates for ion-related energy conversion from natural and daily-life environments.⁶⁻⁹

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Biography:

Guoliang Yang received his doctoral degree from Institute for Frontier Materials (IFM), Deakin University in 2022. He received bachelor's and master's degrees in Environmental Science and Engineering from Dalian Polytechnic University in 2012 and 2015. He is currently an Associate Research Fellow at IFM. He has contributed 36 journal publications, including 6 first/co-first author publications in top-ranked journals, such as ACS Nano and Nano Energy. His research interests focus on the design and functionalization of two-dimensional-material membranes for ion sieving, nanofiltration and clean energy harvesting.

Oral Talks

Surface Reconstructions Optimizations in Energy Conversion Electrocatalysts

Jinxian Feng^{1*}, Chunfa Liu¹, Lulu Qiao¹ and Hui Pan^{1,2}

¹*Institute of Applied Physics and Materials Engineering, University of Macau, Macao, China*

²*Department of Physics and Chemistry, Faculty of Science and Technology, University of Macau, Macao S. A. R., China*

Abstract:

Herein, we study the surface reconstructions optimizations of electrocatalysts for hydrogen evolution reaction (HER), oxygen evolution reaction (OER) and carbon dioxide reduction (e-CO₂RR): (1) The defective FeOOH/Ni hydroxide support on nickel foam (d-FeOOH/Ni hydroxide-NF) has high flexibility of the lattice and tolerates the volume expansion, so the d-FeOOH/Ni hydroxide interfaces are well-maintained, endowing good OER performance. (2) The CoO_x nanocrystalline glass composed of mixed amorphous parts and crystalline domains has high HER performance. The Co oxide skeletons in nanocrystalline glass are stable, and the synergistic effects between the nanocrystalline domains and amorphous matrix benefit the HER kinetics. (3) The Co, Fe dual-metal incorporated Ni hydroxide using NaH₂PO₂ as additive shows high performances for both HER and OER. The in-situ generated active metal improves the accumulation, transportation and activity of protons for HER; and the in-situ generated poor-crystalline hydroxide endows superior charge/mass transportation and kinetics improvements for OER. The results confirm the additive in pre-electrocatalyst fabrication could affect the reconstructions in electrocatalysis. (4) The Cu-incorporated ZnO shows high CO₂-to-CO conversion efficiency. The Cu incorporation prevents the carbonates and hydroxides generation and forms Cu steps, promoting the kinetics of e-CO₂RR. The findings may provide insightful views for electrocatalysts' design and fabrication.

This work was supported by the Science and Technology Development Fund (FDCT) from Macau SAR (0023/2023/AFJ, 006/2022/ALC, and 0111/2022/A2). Multi-Year Research Grants (MYRG-GRG2023-00010-IAPME and MYRG2022-00026-IAPME) from Research & Development Office at University of Macau, and Shenzhen-Hong Kong-Macao Science and Technology Research Programme (Type C) (SGDX20210823103803017) from Shenzhen.

Biography:

Jinxian Feng got his bachelor's degree in chemistry from Sun Yat-sen University at 2015, and got his Ph. D. degree in applied physics and materials engineering from University of Macau at 2023. He is a Ph. D Fellow of University of Macau, Institute of Applied Physics and Materials Engineering currently. His research field covers design, fabrication and mechanism studies of electrocatalysts for energy conversion, like water splitting, CO₂ reduction and N₂ fixation.

Hydrogen Production from Photocatalytic Ammonia Splitting through Single-Atom Catalysis

Jingkai Lin^{1*}, Huayang Zhang¹ and Shaobin Wang¹

¹*School of Chemical Engineering, The University of Adelaide, North Terrace, Adelaide, SA 5005, Australia*

Abstract:

As the most promising clean energy, hydrogen (H_2) is becoming the holy grail of future energy sustainability. Ammonia (NH_3) is an attractive energy carrier with a high H_2 storage capacity (17.8% by weight) and volumetric density ($121 \text{ kg } H_2 \text{ m}^{-3}$ at 10 bar). Unlike other H_2 storage mediums (e.g., CH_4 , CH_3OH), ammonia splitting ($NH_3 \rightarrow 1/2 N_2 + 3/2 H_2$) has zero carbon emission. Importantly, the existing infrastructure for manufacturing, storing, and transporting NH_3 is well-established to support on-site hydrogen production. It is believed that the worldwide energy situation has transitioned into the "ammonia = hydrogen 2.0" era. However, the traditional ammonia cracking process suffered from several limitations, including high operating temperatures of 600 – 850 °C, low energy efficiency, and severe corrosion originating from NH_3 . Herein, we fabricated a series of macroporous carbon nitride-supported single-atom transition metals (TMs-MCN, TMs: Co, Mn, Fe, Ni, Cu) catalyst panels for solar light-driven photocatalytic gaseous NH_3 splitting. Under ambient reaction conditions, the optimized Ni-MCN shows an H_2 production rate of $35.6 \mu\text{mol g}^{-1} \text{ h}^{-1}$, much superior to that of MCN and other TMs-MCN. The enhanced photoactivity of Ni-MCN originates from the presence of Ni- N_4 sites, which improved the optical properties, accelerated charge carrier separation/transfer, and boosted the NH_3 splitting kinetics. The theoretical calculation revealed that introducing Ni- N_4 sites can modulate the electronic structure of MCN, leading to the optimization of binding strength for NH_3 molecules and other reaction intermediates. Our study can provide valuable guidelines for the rational design of single-atom photocatalysts toward energy- and cost-effective photocatalytic NH_3 splitting for H_2 production.

Biography:

Jingkai Lin is currently a Ph.D. student under the supervision of Dr. Huayang Zhang and Prof. Shaobin Wang at the School of Chemical Engineering, the University of Adelaide, Australia. His current research focuses on the development of novel photocatalysts for solar-light-driven energy and environmental applications.

Green Plasma Enhanced Synthesis of Multi-Phase NiMnO₃ Cathode for Aqueous Zn-Ion Batteries

Mitchell Barclay^{1*}, Kudachchige Asanga G. De Alwis¹, Konstantin Firestein¹, Nunzio Motta¹, Deepak Dubal¹ and Kostya (Ken) Ostrikov¹

¹School of Chemistry and Physics and QUT Centre for Materials Science, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

Abstract:

Rechargeable Zn-ion batteries have the potential to address the need for cheap and widely accessible energy storage. Metal doped manganese oxide cathodes are a common and effective choice for Zn-ion batteries. Zn-ion battery development can be advanced by overcoming the poor cycle life that many metal doped Mn Oxide cathodes exhibit. Plasma treated solution (PAW) is used to accelerate the reduction and precipitation of MnO_4^- and nickel acetate (Ni(Ac)) to form a multiphase $NiMnO_3$ electrode with Ni^{2+} and Ni^{3+} doped into the MnO_6 octahedra which exhibits capacitance dominated charge storage mechanisms. The electrode exhibits initial specific capacitance of 60.1 F/g and a capacitance retention of 100.8% after 10,000 cycles and 92.2% after 12,000 cycles. A new layer of nanoflake morphology develops upon the electrode surface during cycling which causes a rapid increase in specific capacitance due to the introduction of electrochemically active surface area and

increase in surface adsorption type charge storage. To better understand the mechanisms of the nanoflake morphology, XPS and Raman spectroscopy is performed on charge/discharge tested electrodes which identifies a decrease in average oxidation state and increase in bond vibrational activity. Finally, we demonstrate the capability of our electrode to be coupled with a Zn metal anode which gives new insight into the compatibility of supercapacitor electrodes as cathodes for rechargeable Zn-ion batteries. The Zn-ion batteries exhibit a peak specific capacity of 331 mAh/g.

Biography:

My name is Mitchell Barclay and I am studying my PhD at the Queensland University of Technology, Brisbane under the supervision of Prof. Kostya (Ken) Ostrikov. The thesis focus is plasma activated matter for improved energy storage electrode materials, with key interests in non-thermal plasma and applications in synthesis of nanomaterials and contributing to the scientific communities knowledge on how non-thermal plasma can benefit many areas of scientific enquiry with a view for developing carbon neutral manufacturing processes.

ROOM B

Session: Biomaterials and Medical Devices

Keynote Talks

Self-Propelled Biocatalytic Nano/Microswimmers

Kang Liang*

School of Chemical Engineering, Graduate School of Biomedical Engineering, Australian Centre for Nanomedicine, The University of New South Wales, Sydney NSW 2052

Abstract:

Micro/nanoswimmers are nano-devices that can convert energy into power to achieve self-propulsion. Compared to ordinary nanoparticles, the driving force of nanoswimmer is their unique advantage. This driving force enables controllable movement with defined direction and speed, allowing nanoswimmers to perform more complex functions.

The application of nanoswimmers for cancer diagnosis and therapy is a new and exciting area of research, which when combined with precision nanomedicine, promises to solve many of the issues encountered by previous development of passive nanoparticles. In this talk, I will highlight some of our recent efforts in the design and engineering of biocatalytic nano/microswimmers through reticular chemistry. By advancing a fundamental understanding of the molecular-level interactions between the soft biocatalysts and functional matrices, we have engineered nano-bio systems with predictable and tuneable physical and chemical properties to address unmet challenges in nanomedicine.

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Biography:

Scientia Associate Professor Kang Liang leads the group of NanoMicroBio Systems at the School of Chemical Engineering and Graduate School of Biomedical Engineering at The University of New South Wales. He received his B.E. and PhD degrees from The University of Melbourne in 2010 and 2014, respectively. He is a former NHMRC Career Development Fellow and currently an ARC Future Fellow. His current scientific interests include the interface engineering of nanostructured materials and nanobiohybrid systems for biomedical and environmental technology.

Self-Powered Flexible Thermoelectric Device for Accelerated Wound Healing

Chongjian Zhou*

¹State Key Laboratory of Solidification Processing, and Key Laboratory of Radiation Detection Materials and Devices, Ministry of Industry and Information Technology, Northwestern Polytechnical University, Xi'an 710072, China

Abstract:

Electrical stimulation emerges as a promising way to accelerate the full-thickness wound healing that remains one of the key challenges in the clinic. However, conventional power generation devices are specially designed and can be accessed by authorized personnel only. Here, we present a flexible and biocompatible thermoelectric device, which can output electricity at the microvolt level from the omnipresent heat in the skin. In mice, we demonstrate the thermoelectric device-induced electricity upregulates the expression of Piezo1-mediated pathways that are associated with tissue regeneration, accelerating the cell migration and proliferation in vitro and healing the wound 6 days faster in vivo. Importantly, the thermoelectric device fast-heals the wound without involving an additional electric circuit such as an amplifier. These advantages will displace the wound healing method and open a new field for thermoelectric application.

Biography:

Chongjian Zhou is currently a professor in the State Key Laboratory of Solidification Processing & Key Laboratory of Radiation Detection Materials and Devices, MIIT, School of Materials Science and Engineering, Northwestern Polytechnical University. He received his Ph.D. degree from the School of Materials Science and Engineering, Xi'an Jiaotong University, in 2016, and worked as a postdoc at Seoul National University in 2017–2021. He focuses on designing functional solid-state materials with extreme thermal properties.

Sustainable Manufacturing and Biomaterials for the Regeneration of Functional (Hard and Soft) Tissues

Sonia Fiorilli*

Department of Applied Science and Technology, Politecnico di Torino, Italy

Abstract:

In the field of biomaterials for tissue regeneration, extensive research efforts are focused on the development of clinical solutions able to overcome the current challenges associated with compromised regeneration of hard and soft tissues. In response to this unmet clinical need, the design of multifunctional devices able to simultaneously target the multiple and interlocked causes (i.e. chronic inflammation, excessive fibrosis, infections) of unsuccessful healing is a key strategy for enabling the recovery of tissue functionality. To this aim, bioactive nanomaterials and natural/synthetic polymers can be synergistically combined through advanced manufacturing technologies, i.e. 3D printing and electrospinning, to provide biomimetic structures and delivery platforms of therapeutics (i.e. drugs, ions, and bioactive molecules) to promote tissue regeneration. This contribution will provide an overview of the research activities focusing on the development of composite 3D scaffolds and flexible nanofibrous patches, as multifunctional solutions to prevent adverse remodelling in bone, skin and cardiac tissues. The developed manufacturing processes mainly rely on formulations of natural-derived functional polymers, such as collagen, chitosan, and alginate, optimized in aqueous-based or non-harmful organic solvents, in order to cope with sustainability criteria. Comprehensive physical-chemical characterization and in vitro/in vivo biological assessments in collaboration with clinicians are reported, highlighting the most relevant achievements, open challenges and future perspectives.

Biography:

Sonia Fiorilli took her PhD in Materials Science and Technology at Politecnico di Torino in 2005. She has consolidated expertise in the synthesis and functionalisation of ceramics and composites for applications in biomedical, energy and environmental sectors. She is/was involved as scientific responsible in several EU-funded collaborative projects related to the development of biomaterials, sustainable manufacturing processes and recycling of critical raw materials. She has been recently selected to receive the 2024 Jubilee Global Diversity Award by the Engineering Ceramics Division of the American Ceramic Society. She has co-authored 114 papers in high-impact peer-reviewed journals (H index = 34)

Enabling Highly Sensitive and Stable Electrochemical Biosensors for Continuous Biomarker Detection

Ming Li^{1*}, Haowei Duan¹ and Yizhou Wang²

¹*School of Mechanical and Manufacturing Engineering, University of New South Wales, Sydney, NSW 2052, Australia*

²*School of Engineering, Faculty of Science and Engineering, Macquarie University, Sydney, NSW 2109, Australia*

Abstract:

Continuous identification and detection of various biomarkers (e.g., nucleic acids, proteins, and small molecules) within biological and environmental samples in a sensitive, stable, and cost-effective manner plays a crucial role in public health, agriculture industry, and environmental monitoring. Electrochemical sensor technology has attracted great interest as a potent way to fulfil this purpose, due to its portability, quantitative read-out, and ease of integration with circuits and microfluidic technologies. However, most currently available electrochemical sensing platforms are limited by insufficient sensitivity, low stability, and/or interference by foreign species, which are significantly hindering their use as a viable

bioanalytical tool for real-world applications. To tackle this critical problem, our group has developed different approaches for electrochemical sensors that enable unprecedented performance in terms of biomarker detection. These include nanocomposite-based coating, molecular probe design, and signal processing optimisation. Our studies have evolved this sensing technology to provide performance improvement while simplifying processes, reducing costs, and shortening time. This will open avenues for the creation of more sensitive and durable real-time monitoring systems in the future, potentially enabling the revolution in medical diagnostics and point-of-care testing.

Biography:

Dr Ming Li is currently an Associate Professor and NHMRC Emerging Leadership Fellow at the University of New South Wales, Sydney, Australia. Her research interests include microfluidics, biosensors, lab-on-a-chip devices, and Micro-Electro-Mechanical Systems (MEMS). She has >70 peer reviewed journal articles published in high-impact journals, such as Cell, Nature Protocols, Biotechnology Advances, Biosensors and Bioelectronics, Small, and Lab on a Chip. Her publications have received over 3,000 citations and an h-index of 31 (Google Scholar).

Oral Talk

Enhanced Hydrogen Therapy by Biomaterial Loaded with Near-Infrared Polymer Dots for Wound Healing

Ziyi Zhang^{1*}, Weijia Wen¹

¹Hong Kong University of Science and Technology

Abstract:

The use of hydrogels as a delivery system has shown great potential due to their ability to encapsulate hydrophilic or hydrophobic therapeutic agents in their 3D polymer network. Nanogels can be constructed through chemical crosslinking or physical self-assembly and can encapsulate a wide range of materials, including small molecules, proteins, nanocarriers and cells. The properties of the nanoscale carrier increase the stability of the loaded cargo and prolong its circulation time. Our previous progress of drug-loaded hydrogel also shown effective sustained-release treatment on inflammatory wound site. In this work, we developed a nanogel system loaded with polymer dots as photocatalysts and vitamin C as a sacrificial electron donor to generate hydrogen for the treatment of nonhealing diabetic wounds. Reactive oxygen species (ROS) in chronic wound prominently delays healing, and sustained hydrogenation to alleviate ROS is hypothesized to promote diabetic wound healing. By red light illumination, the nanogel scavenges ROS in diabetic wounds, augmenting the survival and migration of keratinocytes, promoting angiogenesis, and decreasing inflammatory sites. These effects significantly increase the wound closure rate, indicating that our nanogel loaded with polymer dots represents an effective therapeutic approach for accelerating the healing of chronic diabetic wounds.

Biography:

Ziyi Zhang is a PhD candidate at Hong Kong University of Science and Technology, specializing in the field of functional material fabrication and their application in biomedical fields. She received the 2024 fellowship from Southern University of Science and Technology. Prior to this, she obtained the bachelor's degree in Applied Chemistry from Beijing Institute of Technology and was recognized as an outstanding graduate. With her expertise in

nanomaterials, bio-optics, and therapy methods, she has become a knowledgeable and leading researcher in the field of advanced biomedical materials.

Session: Materials Modelling, Characterization and Data Analytics

Keynote Talks

Theoretical Design of Solid-State Electrolytes

Zhenyu Li*

Key Laboratory of Precision and Intelligent Chemistry, University of Science and Technology of China, Hefei 230026, China

Abstract:

Solid-state electrolytes hold great promise in advancing electrochemical energy storage technology. Simulation techniques play an important role in the design of solid electrolyte materials. In this talk, we first introduce simulation techniques to characterize solid electrolytes. Subsequently, the focus shifts to our recent progresses in enhancing ionic conductivity within bulk electrolytes and investigating ion mobility within the space charge layer (SCL) near charged solid interfaces. In bulk electrolyte, increasing of the defect concentration can often enhance the ionic conductivity. The type of defects also matters. These facts give us opportunities to tune ionic conductivity via defect engineering. Designing a three-dimensional diffusion pathway for Li ions also enhances bulk ionic conductivity. Mechanisms of Li ion diffusion through charged solid interfaces are also discussed.

Biography:

Zhenyu Li is a chair professor of chemistry at University of Science and Technology of China (USTC) and the director of the Key Laboratory of Precision and Intelligent Chemistry. He received his Ph.D. degree in physical chemistry from USTC in 2004. He did postdoc researches at University of Maryland, College Park and University of California, Irvine from 2004 to 2006. Then, he joined USTC as a faculty member. Prof. Li's research interests focus on developing and applying new methods to study microscale mechanisms and properties of materials. Especially, multiscale simulation techniques have been developed in his group to study the mechanisms of graphene growth. In recent year, Prof. Li also put part of his research efforts on quantum computational chemistry. He developed some quantum algorithms for electronic structure calculations for periodic systems. Some wavefunction ansatzes have been proposed to better take the advantage quantum computers.

Green Materials Meets X-ray Absorption Spectroscopy: A Strong and Growing Partnership

Bernt Johannessen^{1,2*}, Jessica Hamilton¹ and Krystina Lamb¹

¹Australian Synchrotron, Australia;

²University of Wollongong, Australia;

Abstract:

X-ray absorption spectroscopy (XAS) is a versatile technique for probing the oxidation states

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

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2. Z. Wu, W. K. Pang, L. Chen, B. Johannessen, Z. Guo, *Batteries & Supercaps* **2021**, *4*, 1547.

Biography:

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

Two-Dimensional Moenes: Structure, Functionalization and Regulation on Physical Properties

Liujiang Zhou^{1,2}

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Key words: MXenes; MOenes; halogenation; quantum phase transition; exciton; nonadiabatic molecular dynamics

Abstract:

The number of semiconducting MXenes with direct band gaps is extremely low; thus, it is highly desirable to broaden the MXene family beyond carbides and nitrides to expand the palette of desired chemical and physical properties. Here, we theoretically report the existence of novel two-dimensional (2D) transition-metal oxides, *i.e.*, $M_{n+1}O_nT_x$ (M = transition metal elements, O = O, S, Se and Te). Single-layer (SL) dititanium oxide Ti_2O MOene, showing an Ising superconducting feature. Specifically, halogenation could induce the transition of metal-to-semiconductor and enable the enhanced light-harvesting ability. In addition, the external strains can induce Weyl fermions via quantum phase transition in Ti_2OX_2 monolayers and Janus ones. 2H- and 1T- Ti_2OF_2 have a direct band gap of 0.82–1.18 eV, showing long carrier lifetimes that is verified by the nonadiabatic molecular dynamics calculations. The quantum spin Hall effect could be observed in $Ti_{n+1}O_nT_x$ ($n=2, 3$). Importantly, we built a 2D

library for the family of MOenes, which provides a novel platform for next-generation nano-devices.

Biography:

Prof. Dr. Liujiang Zhou received his Ph.D. in 2014 from University of Chinese Academy of Sciences. Then he performed postdoctoral research at University of Bremen, Germany and at Los Alamos National Laboratory, USA. He has been a professor at University of Electronic Science and Technology of China since 2019. His research focuses on optoelectronic materials and devices, semiconductor materials, light-matter interaction, computational condensed matter physics & materials, as well as applications of artificial intelligence in materials, growth of crystals, etc.

Rational Design of Low-Dimensional Materials and Database Construction of Two-Dimensional Charged Building Blocks for Functional-Oriented Material Design

Shixuan Du*

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Abstract:

Two-dimensional (2D) materials have attracted considerable attention due to the quantum confinement induced novel physic phenomena, high properties tunability via external field and interface. Therefore, understanding and revealing the structure-composition-property correlation will greatly promote the discovery and design of high-performance 2D materials. In this talk, I will introduce the design strategies to achieve superior properties in the novel 2D monolayer materials, including heteroanionic materials with high carrier mobilities, high Curie temperature magnetic topological nodal line, monochloride with superconductivity and topological metal-organic frameworks, and so on. Moreover, we identify 1028 charged 2D building blocks from Materials Project database using a topological-scaling algorithm. These building blocks host versatile functionalities including super-conductivity, magnetism, and topological properties. We construct layered materials by assembling them considering valence state and lattice mismatch and predict 353 stable layered materials by high-throughput density functional theory calculations. These materials not only inherit their functionalities but also show enhanced/emergent properties compared with their parent materials. This database expands the design space of functional materials for fundamental research and potential applications. Finally, I will talk about a recent work about a stable rhombohedral HfO₂ based ferroelectric material and device.

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Biography:

Shixuan Du contributed many influential works on the nature of molecular assembly, on surface reaction, novel two dimensional atomic crystals, and the growth mechanism of low-dimensional materials. She is the winner of the National Science Fund for Distinguished Young Scholars and the editorial board member of Journal of Physics, Condensed Matter". She got the Award of the Chinese Young Women in Science Fellowship. As a Major Contributor,

she won the 2013's Outstanding Science and Technology Achievement Prize of the Chinese Academy of Sciences. She has published more than 300 journal articles including Science and Nature series.

Theoretical Study on Topological Magnetism in Two-Dimensional Lattice

Yandong Ma*

Shandong University, China

Abstract:

Magnetic skyrmions are topological magnetic quasi-particles exhibiting a whirling spin structure, which have been a prominent topic of condensed matter physics since the first experimental observations of skyrmion lattices in bulk non-centrosymmetric magnet MnSi and thin film Fe_{0.5}Co_{0.5}Si. They can be characterized by spins wrapping a unit sphere, carrying an integer topological charge Q that cannot be changed by a continuous transformation of magnetization. Such topological properties ensure the inherent stability which makes them technologically appealing to be used in future spintronics for information storage and processing. Magnetic skyrmions have been observed experimentally in various bulk and thin film systems. Recently, with the discovery of ferromagnetism in two-dimensional lattice, exploiting magnetic skyrmions in two-dimensional magnetic crystals is at the frontiers of condensed matter physics and material science. In this talk, I will introduce our recent works in this field.

Biography:

Dr Yandong Ma is a professor at the School of Physics, Shandong University. He received his BS and PhD in Physics from Shandong University in 2009 and 2014, respectively. Next, he started work as a postdoctoral researcher at Jacobs University Bremen in Germany with an emphasis on the electronic and magnetic nature of two-dimensional materials. Later, he continued work as a postdoctoral researcher at Leipzig University in Germany working closely with his previous lab. In September 2017, he joined Shandong University as a professor. His current research interests focus on exploring spin and valley physics, including topological magnetism (e.g., skyrmions, bimerons) and valleytronics, through theoretical methods.

New Generation of Reactive Force Field ReaxFF_C-S22 for All-Carbon Materials Across Dimensions and Hybridizations

Yi Liu^{1*} and Fu Liu^{1,2}

¹Shanghai University, Shanghai, China; ²Jining University, Shandong, China

Abstract:

In response to the growing interest in carbon-based materials and their complex allotropes, this research introduces the development of an innovative all-carbon ReaxFF reactive force field, dubbed ReaxFF_C-S22. This force field is specifically designed to accurately model and simulate the diverse array of carbon materials spanning zero to three-dimensional structures, while adeptly handling various carbon hybridizations (sp , sp^2 , and sp^3) and extending to hydrocarbon systems.

The foundation of ReaxFF_C-S22 is built upon a comprehensive dataset derived from quantum mechanics (QM) calculations based on density functional theory (DFT). This dataset

meticulously covers an extensive range of carbon allotropes, embracing their dimensional diversity and the multifaceted nature of carbon atom hybridizations, thereby ensuring the force field's broad applicability and transferability. The robustness of ReaxFF_c-S22 was validated through molecular dynamics (MD) simulations of carbon nanotubes (CNTs) under axial tensile stress and formation of carbon nanowires (CNWs), a long carbon chain encapsulated inside CNTs. Key to our development process was the emphasis on achieving a computationally cost-effective solution without compromising on the fidelity or accuracy of the simulations.

ReaxFF_c-S22 represents a significant leap forward in the dynamic simulation of carbon materials, offering researchers a powerful tool for the design, characterization, and optimization of carbon allotropes and hydrocarbon systems. Its development not only facilitates a deeper understanding of carbon material behaviors under various conditions but also paves the way for the exploration of novel carbon structures and their potential applications, e.g. carbon-hydrogen nano-electronic devices.

Biography:

Prof. Yi LIU obtained his Ph. D. degree at Materials Science and Engineering at Institute of Metal Research in China in 1997. Then he worked at Nagoya University, Japan (1997-2002); Juelich Research Center, Germany (2002-2003); University of Western Ontario, Canada (2003-2005); California Institute of Technology, US (2006-2012). He is a professor at Materials Genome Institute at Shanghai University (2015-) after working at the University of Shanghai for Science and Technology (2012-2015). His current research interests focus on the multi-paradigm materials design for advanced alloys, fuel combustion, and nanomaterials by combining computation (DFT and MD), AI/machine learning, and high-throughput experiment approaches.

Invited Talks

Mechanical Properties and Deformation Behaviour of Graphene/Metal Composites: Insights from Molecular Dynamic Simulations

Che Zhang*

The University of Melbourne

Abstract:

Metal matrix composites (MMCs) have attracted a great deal of research interest due to their superior mechanical and physical properties compared to pure metals. Graphene, known for its exceptional mechanical characteristics, is highly suitable for reinforcement in MMCs. Despite extensive studies on incorporating graphene into metal matrices, systematic research into the mechanical performance of graphene/metal composites at the atomic level remains limited. This study uses molecular dynamics (MD) simulations to explore the mechanical properties and deformation behaviour of graphene/metal composites. The initial research focus of this study is on nano-layered graphene/Cu composites. Findings reveal that increasing the volume fraction of graphene in composites enhances both Young's modulus and tensile strength, although at the expense of a lower yield strain. The composites exhibit a 'negative Poisson's ratio' under uniaxial tension, which is attributable to the enhanced surface effect and the uneven stress distribution at the graphene/Cu interface. Additionally, an asymmetric composite can achieve both positive and negative Poisson's ratios due to

graphene's effective blocking. To address scale limitations, a composite design featuring alternating layers of multilayer graphene and thin Cu films is proposed, maintaining a negative Poisson's ratio even when the total thickness exceeds 100 nm. Another focus of this research is graphene/nanotwinned metal (Gr/nt-metal) composites. Strong strain hardening behaviour is found in Gr/nt-Cu, Gr/nt-Au, and Gr/nt-Ag composites after fast structural transitions. These transitions begin with the propagation of partial dislocations, followed by lattice rotation and the formation of ultrahigh-density twins. Graphene plays an important role in these structural transitions because it provides sites for the dislocation nucleation and acts as a supporting skeleton for lattice rotation. The symmetrical lattice orientation in the nt-metal matrix also promotes a structural transition due to the possibility of dislocation annihilation. However, there is no strain hardening in Gr/nt-Al and Gr/nt-Ni because the wrinkling of graphene cannot induce nucleation of dislocations due to high SF energies of Al and Ni. In addition, the shock response of the Gr/nt-Cu composite is also investigated by MD simulations. Compared to pure nt-Cu and single-crystal Cu, the graphene/nt-Cu composite possesses higher shock resistance and better self-healing ability simultaneously. There is a synergistic effect between graphene and twin boundaries on increasing the plastic sensitivity of the composite at a higher impact velocity, resulting in the larger dislocation density with higher shock resistance. It is expected that this study will fast-track the advancement of graphene-based metal composites, thereby fostering progress in their application domains.

Silicon-Based Anodes for Li Batteries: Thermodynamics, Structural Analysis, and Li Diffusion

Marco Fronzi^{*1} and Amanda Ellis¹ and Eirini Gaudeli¹

**Condensed Matter Theory Group , University of Sydney, Sydney, Australia*

School of Chemical Engineering, University of Melbourne, Melbourne, Australia

Abstract:

Quantum mechanical and machine learning models are used to analyze the properties of silicon composite materials and their impact on lithium-ion batteries' anode performance. The analysis focuses on addressing challenges related to significant volume expansion during lithiation and provides valuable insights into the Gibbs free energy, chemical potentials, and relative stability of LiO and Li⁺ species. Furthermore, the study explores how Li⁺ ions behave in both the primary and secondary phases of the anode, assessing the impact of their formation on ion diffusion. This work highlights the fundamental significance of secondary phases in shaping micro-structural features that impact anode properties, elucidating their contribution to the Li diffusion pathway tortuosity, which is the primary cause for the fracture of Si anodes in Li-ion batteries.

Biography:

Dr. Marco Fronzi is a physicist specializing in computational materials science. Earning his degrees from the University of Rome, he completed his PhD in 2009, concentrating on the catalytic aspects of novel materials. His postdoctoral research in Japan at the National Institute for Materials Science explored materials for energy. Holding roles at Osaka University, the University of Technology Sydney, and Tyndall National Institute, he has delved into the properties of 2D materials and interfaces. Currently, Dr. Fronzi applies theoretical and computational models, including quantum mechanics and machine learning, to predict novel material properties for energy applications.

Focused Ion Beam Sample Preparation for Atom Probe Tomography

Limei Yang*

School of Civil and Environmental Engineering, University of Technology Sydney, Australia

Abstract:

In modern solid materials characterization, focused ion beam (FIB) lift-out is an essential technique for fabricating nanoscale specimens for transmission electron microscopy and atom probe tomography (APT) studies. APT is a powerful technique that can provide quantitative analysis with both high spatial and chemical resolution. This presentation focuses on the applications of APT in material science, geological science and also biological science. A simple and effective sample fabrication methodology using a rotatable micromanipulator in FIB is also introduced. This method enables a quick and precise location of regions of interest and leads to better quality samples with high success rates for APT analysis. The success in preparation will be demonstrated on nanoparticles, nanowire, and thin films, which are typically challenging due to their small sizes.

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Biography:

Dr Limei Yang currently focuses on materials for energy conversion and storage, in the fields of batteries, hydrogen, solar energy, and thermal energy. In particular, she has strong expertise in metal-based hydrogen storage materials. She has worked on various types of materials including metals, alloys, oxides, nitrides, and carbides, which exist in different forms such as nanoparticles, nanowires, thin films, and bulk. Her publications appear in journals such as Nature Energy, Nature Communications, Energy & Environmental Science and Advanced Energy Materials.

Stress-Induced High- T_c Superconductivity in Solid Molecular Hydrogen

Xianqi Song^{1*}, Chang Liu¹, Quan Li¹, Russell J. Hemley², Yanming Ma¹ and Changfeng Chen³

¹Jilin University, China; ²University of Illinois Chicago, USA; ³University of Nevada, Las Vegas, USA

Abstract:

Metallic hydrogen has long been considered the Holy Grail of high-pressure physics that holds the intriguing possibility of realizing room-temperature superconductivity. However, the ultrahigh pressures required for hydrogen metallization impose severe experimental challenges and constraints on synthesis and characterization, leaving large ambiguities and controversies in the interpretation of reported results. Meanwhile, little is known about the influence of nonhydrostatic conditions on its electronic properties at extreme pressures where anisotropic stresses are inevitably present and may also be intentionally introduced. Here we show by first-principles calculations that solid molecular hydrogen compressed to multimegabar pressures can sustain large anisotropic compressive or shear stresses that, in turn, cause major crystal symmetry reduction and charge redistribution that accelerate bandgap closure and promote superconductivity relative to pure hydrostatic compression. Our findings highlight a hitherto largely unexplored mechanism for creating superconducting dense hydrogen, with implications for exploring similar phenomena in hydrogen-rich compounds and other molecular crystals.

Biography:

Xianqi Song is currently working at Jilin University as a Dingxin Postdoc. He graduated from college of physics, Jilin University, China and received the B.S. and the Ph.D. degree in 2016 and 2022, respectively. He has published 17 articles in SCI journals such as PNAS, Nat. Commun., Phys. Rev. Lett., Acta Mater., etc. His research interests include the investigations on high-pressure structures with unusual chemical/physical properties and theoretical design of superhard/superconducting materials. Please see more publication information at his personal website: https://www.x-mol.com/people/xianqi_song?index=3.

Oral Talks

Ferroelectric Domain and Switching Dynamics in Curved In_2Se_3 : First Principles and Deep Learning Molecular Dynamics Simulations

Dongyu Bai^{1*}, Yihan Nie^{1,2}, Jing Shang³, Junxian Liu¹, Yang Yang⁴, Haifei Zhan², Liangzhi Kou¹ and Yuantong Gu¹

¹Queensland University of Technology, Brisbane, QLD, Australia; ²Zhejiang University, Hangzhou, PR China; ³Shaanxi University of Science & Technology, Xi'an, China; ⁴Xi'an Jiaotong University, Xi'an, PR China

Abstract:

Complex strain commonly exists in 2D materials from the fabrication/synthesis process, resulting in significant impacts on the physical and chemical properties [1, 2]. In two-dimensional ferroelectric materials, this deformation can affect the polarization domain, which, in turn, affects their electrical, optical, and thermal properties [3]. Despite these deformations being common in experiments, theoretical investigations are still lacking, primarily due to the absence of effective simulation methods. Here, the effects of bending, rippling, and bubbling on the ferroelectric domains are investigated in an In_2Se_3 monolayer by density functional theory and deep learning molecular dynamics (DLMD) simulations [4]. The DFT results showed that tension (compression) can increase (decrease) the polarization switching energy barrier, leading to an automatic polarization reversal in the bending models. Furthermore, DLMD simulations revealed that the switching dynamics depends

on the magnitude of curvature and temperature, following an Arrhenius-style relationship. Research conducted using complex rippling and bubbling models reveals that lower temperatures and elevated bending strain foster larger domain sizes and longer lifetimes. This study not only provides a promising solution for cross-scale studies using deep learning but also reveals the potential to manipulate local polarization in ferroelectric materials through strain engineering.

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Simulation of Outside Vapor Deposition Process under Various Operational Conditions

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⁴*Institute for Process Modeling and Optimization, Jiangsu Industrial Technology Research Institute, Suzhou 215123, China*

Abstract:

Promoting deposition performance of final product SiO_2 particles is of great importance in the outside vapor deposition (OVD) process for the production of high-quality optical fibers. Two performance indicators for particle deposition, i.e. particle deposition efficiency and mean particle diameter on the target surface, are investigated. In this study, computational fluid dynamics (CFD) was applied to simulate this complex multiphase flow system to obtain typical characteristics of the flow and chemistry such as the velocity and temperature profile etc. The analysis on operational conditions, including the flow rate of raw gas, flow rates of O_2 or H_2 , the mass fraction ratio of SiCl_4/O_2 , and types of the carrier gas, was conducted. The predicted results indicate that there is an optimum flow rate of raw gas to yield the peak deposition efficiency. The particle deposition efficiency declines as flow rates of O_2 or H_2 rises. Furthermore, using O_2 as carrier gas yields larger deposition efficiency compared to H_2 and N_2 , which present less uniform deposition of silica particles on the target surface. This analysis provides a good understanding of impacts of the operational parameters on SiO_2 particle deposition, which are crucial for the process optimization and product quality control.

Biography:

Jun He obtained her Bachelor's degree majoring in Bioengineering, and her Master's degree in the field of Environmental Engineering. During her PhD study, the journal paper titled "Eulerian-Eulerian modeling of the formation and deposition of SiO₂ in the outside vapor deposition process" was published. She is currently a PhD student under the Southeast University-Monash University joint award program. Her current research interests involve complex phenomena in OVD deposition process.

Light-Switchable Biocatalytic Covalent–Organic Framework Nanomotors for Aqueous Contaminants Removal

Jueyi Xue^{1,2*}, Mengnan Zhang^{1,2}, Joel Yong^{1,2}, Qianfan Chen³, Joseph Wang⁴, Jiangtao Xu^{1,2}, and Kang Liang^{1,2,3}

¹*School of Chemical Engineering, The University of New South Wales, Australia*

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Abstract:

In the realm of water remediation applications, the utilization of cutting-edge green materials, particularly self-propelled nanomotors, with their ability to autonomously navigate and perform specific tasks on the nanoscale, emerges as a revolutionary approach, harnessing the power of environmentally friendly nanotechnology to efficiently and sustainably address water pollution challenges. On the other hand, light displays remarkable adaptability in controlling the movement of nanomotors, combined with the ease of acquisition and remote control, enhance the appeal of light-driven nanomotors for a wide array of practical applications. Herein, we present a biocatalytic nanomotor based on a covalent–organic framework (COF) via green synthesis that demonstrates intelligent and switchable motion triggered by a blue-to-red light switch, named as CAT-PAH@RT-COF-1. The resulting CAT-PAH@COF nanomotor exhibits intelligent light-responsive motion, featuring an on/off switch between blue and red light at a low H₂O₂ concentration of 50 mM (0.02 wt %). As a proof-of-concept for its applications, a significant improvement of contaminant removal in aqueous environments was demonstrated by this enhanced mobility. Consequently, when exposed to blue light, the nanomotor significantly enhances the removal of contaminants in aqueous solutions due to its elevated mobility. Conversely, it effectively deactivates its motion and contaminant removal upon exposure to red light. This study explores the heterogeneous assembly strategy of the COF-based nanomotor and its light-controlled propulsion performance and provides a novel strategy for the regulation of movement, offering valuable insights for the design and practical applications of nanomotors in green materials and their environmental applications.¹

Biography:

Jueyi Xue is a PhD candidate supervised by A/Prof. Kang Liang at School of Chemical Engineering, UNSW Australia. She received her MEng degree in Biomedical Engineering at UNSW in 2020 and continuing her academic journey toward a doctoral degree. Her research interest focuses on bio-nanohybrids and their applications in environmental and biomedical engineering based on metal-organic-frameworks (MOFs) and covalent-organic-frameworks

(COFs). Her work underscores a commitment to advancing the frontier of knowledge at the nexus of bioengineering and nanotechnology for a more sustainable and healthier future.

The work has been published in *Nano letters*.

Xue, J.; Zhang, M.; Yong, J.; Chen, Q.; Wang, J.; Xu, J.; Liang, K. Light-Switchable Biocatalytic Covalent–Organic Framework Nanomotors for Aqueous Contaminants Removal. *Nano Lett* **2023**. <https://doi.org/10.1021/acs.nanolett.3c03766>.

ROOM C

Session: Electronic Materials

Keynote Talks

Interfacial Synthesis of 2D Framework Electronic Materials

Renhao Dong*

Key Laboratory of Colloid and Interface Chemistry of the Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, 250100 Jinan, China.

Abstract:

In our work, we have employed interfacial chemistry toward the controlled synthesis of conductive 2D framework materials (2DFMs) with precision structures.^[1] For instance, we demonstrated the synthesis of 2D conjugated metal-organic framework (2D c-MOF) at the air-water or liquid-liquid interfaces. The 2D c-MOFs feature with stacked layers and possess unique electronic properties, such as full π delocalization, narrowed band gaps and high conductivity, which render 2D c-MOFs as advanced electronic materials.^[2] One representative iron-bis(dithiolene) 2D MOF exhibited as a p-type semiconductor with a band-like transport and high mobility.^[3] Owing to their conductivity, the 2D c-MOFs have shown potential for transistors, photodetectors, sensing, magnetics, and energy storage and conversion.^[4] In addition, we have also synthesized highly crystalline 2D polymers on the water surface. For instance, we have employed a surfactant-monolayer-assisted interfacial synthesis (SMAIS) method to prepare 2D polymers,^[5] like 2D polyimides, 2D polyimines and boronate ester 2D polymers, which exhibit few-layers and micrometer-sized single-crystalline domains, which have been utilized as active layers for optoelectronics and memory devices. As another typical example for SMAIS, we have developed charged 2D polymer single crystals through an irreversible Katritzky reaction under pH control, which could act as an anion-selective membrane for osmotic energy generation, offering a high chloride ion selectivity.^[6] In our latest work, we have developed BBL-based 2D conjugated polymer film, which exhibited high THz mobility over $10^3 \text{ cm}^2/\text{Vs}$.^[7] We expect that our research could push the development of conductive 2DFMs for electronics (FMtronics).

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Biography:

Dr. Renhao Dong received his doctor's degree on physical chemistry in 2013 in Shandong University. Then, he joined Max Planck Institute for Polymer Research as a Humboldt postdoctor. Since 2017, he has worked as a group leader and then a TUD Investigator, PhD supervisor, leading an international group in Dresden University of Technology (TUD). Since 2021, he has worked as a full Professor in Shandong University. His current scientific interests focus on functional interface and organic 2D crystalline materials. Thus far, Dr. Dong has published over 120 peer-reviewed articles which have attracted more than 12000 citations with h-index of 50.

Engineering Topological States in Two-Dimensional Antiferromagnets

Chengwang Niu* and Ying Dai

Shandong University, China

Abstract:

Magnetic topological states open up exciting opportunities for exploring fundamental topological quantum physics and innovative design of topological spintronics devices. A famous example is the antiferromagnetic (AFM) topological insulator (TI) state, which, however, was still not observed in two dimensions. Using a tight-binding model and first-principles calculations, we show that an AFM TI can emerge in two dimensions with the nonsymmorphic symmetry that combines the twofold rotation symmetry and half-lattice translation [1]. In addition, we put forward that the stacked Chern insulators with opposite chiralities offers a strategy to achieve the gapless helical edge states in two dimensions, and a highly robust magnetic topological insulator phase, which remains intact under both ferromagnetic and antiferromagnetic configurations, can emerge in two dimensions as well [2,3]. The nontrivial topologies of the proposed magnetic insulating states are confirmed by the direct calculation of the spin Chern number, Wannier charge centers, and the nontrivial topological edge states. Our results improve the understanding of the relationship between band topology and magnetic structure in two-dimensional materials.

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Optomechanics Induced Phase Transition Under Light

Jian Zhou*

Xi'an Jiaotong University, China

Abstract:

Two-dimensional materials have shown tremendous interesting features with large surface area to volume ratio. Hence, they are optically addressable and accessible. In this talk, I will discuss some recent theoretical predictions, focusing on the terahertz optics driven phase transition of ferroelectric materials, including their geometric phase transition and electronic responses. The specific materials that I will be focusing on are group IV monochalcogenide compounds (such as SnSe, SnS, GeS, GeSe, SnTe, etc.), in bulk and two-dimensional phases. Non-contacting optical readout/write with focused laser would be preferable in many circumstances. We use first-principles density functional theory calculations to theoretically and computationally illustrate an optomechanical strategy to inducing geometric phase transitions, which uses a linearly polarized laser with selected frequency. Such ultrafast diffusionless martensitic phase transition holds the essence of next generation communication technology.

Biography:

Jian Zhou, Professor at School of Materials Science and Engineering, Xi'an Jiaotong University. Zhou received Bc.S. (2008) and Ph.D. (2013) at Peking University in Theoretical Mechanics, followed by Postdoctoral Association position at Virginia Commonwealth University and Massachusetts Institute of Technology (2013-2018). His current research interests mainly focus on first-principles calculations of nonlinear optics of condensed matter materials, photoinduced material structures, and topological phase transitions. So far, he co-authored over 100 papers in PNAS, PRL, Nano Letters, etc. These papers have been cited more than 6,000 times, with an h-index of 33, and was selected as "Elsevier China Highly Cited Scholar".

Interlayer Magnetoelectric Coupling in Van Der Waals Structures

Wei Wei*

School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China

Abstract:

We propose a novel method to intrinsically realize the nonvolatile electrical control of noncollinear antiferromagnetism, and translate our idea to concrete van der Waals VI_2 bilayers from the first-principles calculations. In VI_2 bilayer systems, we unravel that the sliding ferroelectricity couples strongly to the spin spiral chirality of each VI_2 monolayer, to which we refer as the spin spiral chirality–sliding ferroelectricity locking effect. In this view, flexibly electrical switch of the noncollinear antiferromagnetism can be realized via interlayer sliding. Our work therefore opens a new direction for the study of type-II multiferroic materials in two dimensions.

Engineering Diamond Surfaces for Quantum Diamondtronics

Dongchen Qi*

School of Chemistry and Physics, Queensland University of Technology, Brisbane, Queensland 4001, Australia

Abstract:

Despite being a bona-fide bulk insulator, diamond develops an intriguing two-dimensional (2D) *p*-type surface conductivity when its surface is terminated by hydrogen and exposed to appropriate surface adsorbate layer such as atmospheric water as a result of the surface transfer doping process. Consequently, the surface of diamond presents a versatile platform for exploiting some of the extraordinary physical and chemical properties of diamond, leading to applications such as chemical/biological sensing and the development of high-power and high-frequency field effect transistors (FETs).

In this talk, I will describe our recent work on the surface transfer doping of diamond by transition metal oxides (TMOs). Specifically, I will show that by interfacing diamond with MoO_3 or V_2O_5 a 2D hole conducting layer with metallic transport behaviours arises on diamond. The 2D hole layer affords a surprisingly large spin-orbit interaction giving rise to exotic quantum coherent spin transport properties as revealed by low-temperature magnetotransport. The spin transport can be further tuned by an external electric field in a metal-oxide-semiconductor FETs (MOSFETs) architecture. Lastly, solution-processible approaches for the formation of ultrathin metal-oxide layers on diamond to enable *p*-channel diamond surface electronics are also explored.

Biography:

During 1999 to 2003 Dr. Qi studied physics in Peking University for his undergraduate education before he moved to Singapore. After receiving his PhD degree in surface science from the National University of Singapore in 2009, he spent another two years as a research fellow at the same institute. In 2012, he joined the Institute of Materials Science and Engineering (IMRE) as a staff scientist working on organic electronic devices. He took up a faculty position as a lecturer in physics at La Trobe University in 2013. In 2017, Dr. Qi was awarded the prestigious ARC Future Fellowship to develop high-performance diamond surface electronics and quantum devices. In 2018, He joined the Queensland University of Technology as a Senior Lecturer and was promoted to Associate Professor in 2020. Dr. Qi's research interests lie in the area of experimental condensed matter physics and material physics, focusing on creating, understanding, and controlling at nanoscale the surfaces and interfaces of functional materials to develop new technologies and material platforms for the next-generation devices.

Non-Hydrostatic Pressure Induced Superconductivity in Diamond and Solid Molecular Hydrogen

Quan Li*

Jilin University, China

Abstract:

Diamond is a prototypical ultrawide band gap semiconductor, but turns into a superconductor with a critical temperature T_c of 4 K near 3% boron doping. Here we unveil a surprising new route to superconductivity in undoped diamond by compression-shear deformation that induces increasing metallization and lattice softening with rising strain, producing phonon mediated T_c up to 2.4–12.4 K. This finding raises intriguing prospects of generating robust superconductivity in strained diamond crystal, showcasing a distinct and hitherto little explored approach to driving materials into superconducting states via strain engineering. We show by first-principles calculations that solid molecular hydrogen compressed to

multimegabar pressures can sustain large anisotropic compressive or shear stresses that, in turn, cause major crystal symmetry reduction and charge redistribution that accelerate bandgap closure and promote superconductivity relative to pure hydrostatic compression. Our findings highlight a hitherto largely unexplored mechanism for creating superconducting dense hydrogen, with implications for exploring similar phenomena in hydrogen-rich compounds and other molecular crystals.

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- [3] X. Song, C. Liu, Q. Li, R. J. Hemley, Y. Ma, and C. Chen, Proc. Natl. Acad. Sci. USA 119, e2122691119 (2022).

Biography:

Quan Li, Au-Chin Tang Scholar Distinguished Professor in Jilin University, awarded Ph.D in condensed matter physics, Jilin University (2011) and worked as a postdoctoral researcher at University of Nevada, Las Vegas, USA (2011~2013). He received Distinguished Young Scientists Fund (NSFC) in 2023, Excellent Young Scientists Fund (NSFC) in 2016, the First-Class Prize of Natural Science Award of Jilin Province (the 1st awardee) in 2022, the Second Prize of National Natural Science Award in 2015 (the 4th awardee), Excellent Young Scientist Award in 19th China High Pressure Conference. He has published 100+ refereed papers in journals such as Phys. Rev. Lett., J. Am. Chem. Soc., PNAS, Nature Comm., et al. His research focuses on (1) structure and physical properties of novel superhard materials; (2) physical properties of functional materials under non-hydrostatic pressure.

Manipulating the Structure and Properties of Two-Dimensional Carbon-Nitrogen Materials

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²Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Soochow University, 199 Ren'ai Road, Suzhou, 215123, Jiangsu, P. R. China.

³Centre for Theoretical and Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, QLD, 4072, Australia.

Abstract:

Two-dimensional (2D) carbon nitrides have garnered extensive attentions due to their potential applications in semiconductor devices, high-performance catalyst, lithium-ion batteries, supercapacitors, fuel cells, hydrogen storage materials, etc. However, the practical application of these materials in these fields faces challenges in controlled synthesis. The carbon nitride materials prepared in current experiments generally exhibit low nitrogen doping concentration and a mix of different types of nitrogen atoms, which limits their broader application. Based on first-principles calculations, we have conducted a comprehensive study on the structural and property control of two-dimensional carbon nitride materials (C_{1-x}N_x).

In this presentation, we will discuss: (i) the stable structures inherent in $C_{1-x}N_x$, and the ways in which these structures can be engineered through the adjustment of experimental conditions, including the C/N raw material ratio, hydrogen pressure, and temperature; [1] (ii) the coexistence of graphitic and pyridinic nitrogen in $C_{1-x}N_x$ and its impact on electrocatalytic activity; [2] and (iii) controlling the band gap of bilayer C_3N by altering the interlayer stacking and applying an external electric field. [3] These theoretical studies provide important guidance for the precise synthesis of two-dimensional carbon nitride materials and their application in the field of electronic devices.

References:

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[3] W. Wei, Q. Yuan,* et al. *Nat. Electron.* 2021, 4, 486.

Biography:

Qinghong Yuan received her PhD in Theoretical Chemistry from the Chinese University of Hong Kong in 2010. From 2010 to 2012, she was engaged in postdoctoral research at Hong Kong Polytechnic University. In August 2012, she joined East China Normal University as an associate professor and was promoted to a full professor in 2015. Qinghong Yuan received a DECRA fellowship from the Australian Research Council in 2016. Her research interest focuses on theoretical study of low-dimensional nanomaterials. She has published more than 80 peer-reviewed papers in high impact journals, including *Nat. Mater.*, *Nat. Electron.*, *Nat. Commun.*, *J. Am. Chem. Soc.*, *Phys. Rev. Lett.*, etc.

Invited Talks

Computational Design of Novel Nanomaterials

Zhenpeng Hu*

School of Physics, Nankai University, China

Abstract:

Based on the basic concepts in solid physics, a computational design of nanomaterials has been performed. By substituting the repeating unit with various polyhedrons in the lattice, nanomaterials with different properties can be obtained. Following this protocol, carbon-based and boron-based nanomaterials with novel physical properties have been designed, including materials with tunable flat bands and high order von Hove singularities, ultrawide gap semiconductor, node-line semimetal, and so on.

Biography:

Zhenpeng Hu got his B. S. (2002) and Ph. D (2008) at University of Science and Technology of China (USTC). Then, he went to University of California, Santa Barbara (UCSB) to do his postdoctoral research. On December 2011, he joined Nankai University as an associate professor. He was promoted to a full professor in 2017 and supported by Fok Ying Tung Education Fund between 2016 and 2019. He has been engaged in the research on the electronic structure and physical properties of materials for a long time, publishing over 100 peer-reviewed papers that cited over 6000 times (H-index of 42).

2D Materials as Hardmasks

Ya-Ping Hsieh*

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Abstract:

This presentation introduces our recent research on new 2D materials synthesized by confined CVD and their application, with a focus on semiconductor fabrication processes. Photolithography is a key obstacle to increasing the density of electronic devices.

We have discovered that bilayer graphene could turn into fluorographene/graphene stacks when exposed to CF₄ plasma, which exhibits near-ideal etch selectivity in silicon dry-etching processes. Based on this advance, bilayer graphene was adopted as a hard mask for photolithographical patterning of semiconductors. The atomic thickness of our hard mask can improve the achievable resolution of the resulting pattern and we demonstrated nanometer-scale resolution of the bilayer graphene mask in a double patterning process.

Moreover, we utilized graphene's natural wrinkles to pattern transfer such nanostructures to transition metal dichalcogenides (TMDCs). This subtractive pattern transfer process allows us to fabricate TMDC nanoribbons with an aspect ratio of up to 7000 and nanometer-width with unprecedented density. This research opens up new possibilities for creating nanostructures with greater precision using 2D materials.

To extend our findings towards commercially significant reactive ion etching processes, we require a 2D material with higher hardness and chemical inertness than graphene. I will introduce the appeal of two-dimensional tungsten nitrides (W₅N₆) for this purpose. We demonstrate the first successful synthesis of W₅N₆, an ultrahard semimetal which could provide a new route towards a 2D hard mask for improved efficiency and accuracy of the lithography.

Biography:

Ya-Ping Hsieh is an associate research fellow at, Academia Sinica Taiwan. She is also an adjunct professor at many universities in Taiwan, such as National Chung Cheng University and National Taiwan University. Ya-Ping has organized a couple of international conferences and is constantly an organizing committee in Taiwan's annual Physical Society meetings. Her research focuses on novel 2D material synthesis using confined CVD methods and exploring their applications in electronics. In the last ten years, She has published three book chapters, two patents, and ~100 original SCI papers.

Session: Materials Science and Engineering

Keynote Talks

Lubrication and Mechanism of Carbonate at High Temperature

Long Wang^{1*} and Weimin Liu¹

¹Center of Advanced Lubrication and Seal Materials, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi, 710072, PR China

Abstract:

Many industrial processing operations involve hot metal forming. In the rubbing counterparts

of the interacting surfaces at high temperature, lubrication is crucial in reducing friction and wear for the hot metal forming process, the benefits include a reduced energy consumption, a reduced tool/component wear and a longevity of moving machine parts. Graphite based lubricants has been widely used. However, energy and environment concern require new and “white” lubricant to replace the conventional graphite or oil contained lubricant. At high temperatures and under high shear conditions, some inorganics transition from the solid into a semi-liquid phase (melt) can occur, which can lubricate the sliding interface.

Alkaline carbonate is a water-soluble environmental-friendly salt, which has a wide range of applications in glass manufacturing, food additives, cooking etc. They melt in the temperature range from 750-890 °C, which is likely to offer lubrication for the hot metal forming. This work reports the potential application of alkaline carbonate as an environmentally friendly and inexpensive high-temperature lubricant for hot metal rolling of steel. Its performance was evaluated by the ball-on-disc tribo-tests at high-temperatures. Significant reduction of friction and wear was achieved, which was attributed to the tribo-induced melting of sodium carbonate at the sliding interface, which acted as a liquid lubrication layer and formed a shear-induced nano-gradient tribofilm structure. The sodium carbonate melt was readily sheared and produced low friction and negligible wear. The nano-gradient tribofilm structure which formed under sliding inhibits cracking and spalling, resulted in a low wear due to strain delocalization.

Keywords: Hot metal forming, Lubricant, Nano-gradient tribofilm, Alkaline carbonate, Tribology

A Promising Experimental Platform: *In-situ* Magnetization Measurement Setup Under Magnetic Field

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¹State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, China;

²Univ. Grenoble Alps, LNCMI, F-38000 Grenoble, France;

Abstract:

A new promising experimental platform has been developed for studying the solidification of undercooled molten materials and simultaneously measuring their magnetization under strong magnetic fields. This platform allows for in-situ measurement of the magnetization of undercooled melts and investigation of non-equilibrium solidification of metals and alloys in magnetic fields. The major advantages of this platform are as follows: Firstly, it enables the generation of large undercooling in high magnetic fields using a combination of glass fluxing technique and cyclical superheating and supercooling method, which can achieve similar maximum undercooling levels as the traditional method without magnetic fields. Secondly, it offers precise control over the thermal history of the samples, including linear heating and cooling rates with high accuracy. Lastly, the temperature and magnetization measurement system is fast and online, making it suitable for studying both structural transitions in the liquid state over a wide temperature range (overheated and undercooled states) and solid state phase transformations. Several typical applications of this platform will be outlined during the talk.

Keywords: Magnetic field; Experimental platform; Structural transitions; Phase transformation.

Biography:

Yixuan He, an associate professor and doctoral supervisor, is primarily engaged in research on material preparation and control of structural properties under the influence of strong magnetic field. He has led or participated in numerous national-level research projects, including the National Natural Science Foundation, major scientific instrument development projects, and national key research and development programs. He has published over 50 SCI papers and has been granted more than 10 national invention patents.

Bulk Nanostructured Metallic Materials by Advanced Rolling Process

Lihong Su*

School of Mechanical, Materials, Mechatronic and Biomedical Engineering, University of Wollongong, Australia

Abstract:

Bulk nanostructured metallic materials (BNMMs) have attracted wide research interest due to their unique physical and mechanical properties. In comparison with conventional fabrication methods, such as gas condensation and ball milling, severe plastic deformation (SPD) methods have great advantages in avoiding residual porosity and impurities during fabricating bulk nanostructured materials. Advanced accumulative rolling process, as one of the most popular SPD techniques, has attracted the growing interest because it has the most potential in producing large scale product for practical applications. Microstructural features and mechanical properties of several representative BNMMs have been comprehensively investigated in this study, and their potential applications have also been discussed.

Biography:

Dr. Lihong Su received her PhD from University of Wollongong, Australia, where she is currently working as a senior lecturer. She has won several prestigious awards based on her excellent research record, including France-Australia Science Innovation Collaboration (FASIC) fellowship, Japan Society for the Promotion of Science (JSPS) fellowship, and Australian Discovery Early Career Researcher Award (DECRA) fellowship. She has published more than 70 highly cited research papers in peer reviewed journals and delivered more than 10 invited or keynote talks in high-qualified international conferences. Her research interests include design, manufacturing and characterizing novel high-performance metallic materials and composites for extreme conditions, such as light-weight aluminum and titanium alloys, high-strength steels, and high entropy alloys.

Discovery of Two-Dimensional Organic Polymer Photocatalysts for Overall Water Splitting under Visible Light through Theory

Xiaojun Wu*

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Abstract:

Using solar energy to split water to prepare hydrogen and oxygen is an important way to obtain clean hydrogen energy and solve energy and environmental problems. In recent years, organic polymers have emerged as emerging materials for photocatalytic total water

decomposition due to their optical and electronic structures that can be designed and modulated at the molecular level. How to modulate and design the energy band structure of organic polymers to achieve total photolysis of water under visible light is one of the key issues in this field. We applied the first-principles electronic structure calculation method to effectively regulate the valence band and conduction band electronic structures of two-dimensional organic polymers from a molecular perspective by selecting the molecular types of connecting groups and nodes, on the basis of which we found the carbon-nitrogen-based two-dimensional conjugated porous polymer materials that can be used for visible-light catalysis of oxygen production, and the two-dimensional organic polymers that can be used for the total decomposition of water in visible light, and experimental studies are in agreement with theoretical predictions. A series of 2D organic polymer photocatalytic materials that can be used for the total decomposition of water were predicted by screening a database of 2D organic polymers. Finally, we developed a strategy to design 2D organic polymer photocatalytic materials based on functional molecular motifs to achieve overall water splitting under visible light irradiation.

Biography:

Xiaojun Wu, professor of computational materials and chemistry at the University of Science and Technology of China (USTC). He received her B.S. and Ph.D. degrees from the Department of Chemical Physics, University of Science and Technology of China (USTC) in 1996 and 2005, respectively, and was a postdoctoral researcher at the University of Nebraska, Lincoln, USA, from 2005 to 2010. His research area is theoretical and computational chemistry, and his research interests include theoretical design of materials and physicochemical processes at surface interfaces.

Influence of Ru on the Thermo-Mechanical Fatigue Deformation Mechanism of a 4th Generation Nickel-Base Single Crystal Superalloy

Guang Xie*

Chinese Academy of Sciences, China

Hierarchical Mesoporous Superparticles: Precise Synthesis and Applications

Zaiwang Zhao^{1,*}, Guangmei Jiang¹, Xiao Han¹, Xiankai Fan¹, Yujuan Zhao¹ and Dongyuan Zhao^{1,2}

¹College of Energy Materials and Chemistry, Inner Mongolia University, Hohhot, China.

²Laboratory of Advanced Materials, Fudan University, Shang Hai, China

Abstract:

Hierarchical mesoporous materials are vital in many fields such as photocatalysis and energy storages, but the precise synthesis remains a great challenge. Some typical works reported by our groups listed below: i) an ultra-stable single micelle was obtained *via* a thermodynamic method, and the ultra-small organic-inorganic nanohybrids (<50 nm) with good monodispersity and uniformity were synthesized, involving SiO₂, TiO₂, ZnO, Ag *etc.*; ii) various "earth-satellites" type superstructures were synthesized through a single-micelle based an interface super-assembly strategy. In this structure, single micelles were regularly arranged on the surface of the spherical SiO₂ substrates in a quasi-ordered hexagonal

manner. 3) mesoporous carbon superstructures with a monolayer of spherical mesopores (22 nm) on the surface of center hollow (300 nm) were synthesized by a facile monomicelle interface confined assembly strategy. At the same time, there was a small pore (4.0-4.5 nm) on the inner surface of each spherical mesopore, making it totally interconnected. This superparticle exhibited a high specific surface area ($685 \text{ m}^2\text{g}^{-1}$) and excellent underwater hydrophilicity. In addition, the precise control of the number of mesopores (70-360) has been achieved for the first time, which is unachievable by the traditional methods. Finally, the efficient catalytic performance of this mesoporous superparticle was demonstrated.

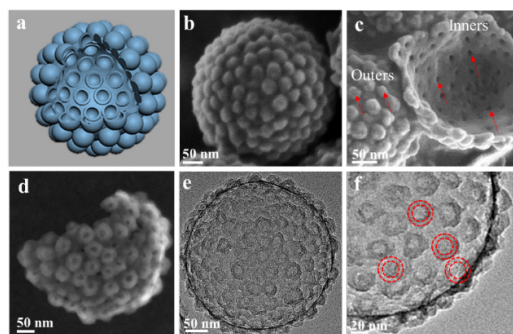


Fig. 1 Mesoporous superstructures with monolayered spherical mesopores.

Key words: mesoporous materials, monomicelle, assembly, catalysis, applications

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- [4] [Zaiwang Zhao](#), Dongyuan Zhao*, et al. (2022) J. Am. Chem. Soc. 144, 11767.
- [5] [Zaiwang Zhao](#), Dongyuan Zhao*, et al. (2021) Adv. Mater. 2021, 33, 2100820.

Biography:

Prof. Zaiwang Zhao, Inner Mongolia University, doctoral supervisor, a young researcher in Academician Zhao Dongyuan's team. Research interest: Synthesis and energy applications of functional mesoporous materials. He has hosted several projects, including the National Natural Science Foundation of China. As a corresponding or first author, more than 50 papers have been published in famous journals, such as *Nat. Protoc.*, *Sci Adv.*, *J. Am. Chem. Soc.*, *Adv. Mater.*, *Environ. Sci. Technol.*, etc. And one paper has been selected as one of the "100 papers with the most international influence". The total number of citations for the paper is over 6000.

Invited Talks

New Technology to Degrade PFAS

Cheng Fang*, Yunlong Luo and Ravi Naidu

Global Centre for Environmental Remediation (GCER), University of Newcastle, Callaghan NSW 2308, Australia.

Cooperative Research Centre for Contamination Assessment and Remediation of the Environment (CRC CARE), University of Newcastle, Callaghan NSW 2308, Australia.

Abstract:

Electrochemical advanced oxidation process (EAOP) has demonstrated significant potential to degrade per- and polyfluoroalkyl substances (PFAS) which is still a big challenge. However, towards the widespread application, EAOP is still impeded by the declined long-term performance and the limited service life of electrodes. This study introduces a novel approach by investigating the impact of polarity reversal (PR) of the applied current on the electrochemical degradation of PFAS including aqueous film-forming foam (AFFF) samples. An electrochemical cell equipped with two titanium sub-oxide (Ti₄O₇) electrodes is used for the experimental investigation. The results indicate 6-hour direct current (DC) operation causes fouling and ageing of the electrode (anode) such as the formation of titanium oxide (TiO₂). Fouling/ageing is effectively mitigated when the PR current is applied. PR is also found to enhance the defluorination of PFAS, likely attributed to improved mass transfer and an observed reduction in electrode fouling/ageing towards prolonged service life. The investigation also suggests that PR can help to reduce the energy consumption by ~13%. Overall, the application of PR emerges as a promising and practical strategy to augment the electrochemical degradation of PFAS, addressing critical issues related to electrode stability and longevity.

Biography:

A senior researcher in the fields of SERS (surface-enhanced Raman scattering), AIE (aggregation induced emission), electrochemistry, nano-device (nanowire, nanogap, nanomembrane etc.), environmental monitoring and remediation using advanced electrochemistry, nano-materials, lab-on-chip etc. Recently focusing on PFAS, micro-/nanoplastics.

Ultrastrong Nanotwinned Titanium Alloys through Additive Manufacturing

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⁶College of Engineering and Computer Science, Australian National University, Canberra, ACT 2601, Australia

⁷Center for the Accelerated Maturation of Materials, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH 43212, USA

Abstract:

Additive manufacturing is leading a new era in metal fabrication across aerospace, automotive,

biomedical and energy sectors due to its design freedom that can fabricate almost any geometrical part. Titanium alloys are presently the leading additively-manufactured metal components for the aerospace industry. However, most commercially available titanium alloys made by additive manufacturing do not have satisfactory properties for many structural applications. In this talk, we will present our recent breakthrough that ultrastrong and thermally stable titanium alloys can be produced by additive manufacturing, which may be directly implemented in service. As demonstrated in a commercial titanium alloy, after simple post heat treatment, adequate elongation and tensile strengths over 1600 MPa are achieved - resulting in the highest strength-to-weight among all AM alloys to date. The excellent properties are attributed to the unusual formation of dense, stable and internally-twinned nanoprecipitates, that are rarely observed in the traditionally processed titanium alloy. These nano-twinned precipitates are shown to originate from a high density of dislocations with a dominant screw character and formed from the AM process. The work herein paves a way to fabricate structural materials with unique microstructures and excellent properties for broad applications.

Biography:

Dr. Yuman Zhu currently serves as the Deputy Director of the Monash Centre for Additive Manufacturing (MCAM). He is also a Future Fellow of Australia Research Council (ARC) and a Senior Lecturer within the department of Materials Science and Engineering at Monash University. His research interests involve investigating the additive manufacturing process of metallic materials, and application of advanced electron microscopy techniques to study the rapid solidification and phase transformations associated with the AM process, aiming to establish microstructure / mechanical property relationships and advance the application of AM.

Designing Oxygen Evolution Electrocatalysts by Leveraging the Lattice-Oxygen Mediated Mechanism

Xiaomin Xu^{1*} and Zongping Shao¹

¹WA School of Mines: Minerals, Energy and Chemical Engineering (WASM-MECE), Curtin University, Australia

Abstract:

Water electrolysis powered by renewables-generated electricity represents one of the simplest approaches to production of green hydrogen, which, however, is largely impeded by its insufficient efficiency associated with the sluggish kinetics of the half-reactions involved, in particular, the oxygen evolution reaction (OER) on the anode side. Understanding the reaction mechanisms has proven to be instrumental in developing better OER catalysts. It is recently found that the bulk lattice oxygen of a catalyst could participate in the OER via a so-called lattice oxygen-mediated mechanism (LOM), which can bypass the scaling relationships that are known to constrain the OER activity in the conventional adsorbate evolution mechanism (AEM). Here, we showcase, by designing model catalysts based on perovskite oxide structures, how lattice oxygen can directly participate in the OER and how better catalysts utilising the LOM mechanism can be developed using materials engineering strategies like doping, defect engineering, and compositing. We further show the application of the LOM-based perovskite OER catalysts in practical devices like anion-exchange membrane water electrolyzers which delivered appreciable activity and stability when operated under elevated temperatures. We expect that these new insights into OER catalysis can facilitate the development of the water

electrolysis technology for green hydrogen production.

Biography:

Xiaomin Xu obtained his Ph.D. in chemical engineering from Curtin University, Australia. He is currently a research associate at Curtin University. His research interests are mainly focused on the development of functional materials for applications in electrochemical energy storage and conversion including water splitting, zinc-air batteries, and CO₂ electroreduction.

Oral Talk

Carrageenans as Sustainable Water-Processable Binders for High-Voltage NMC811 Cathodes

Ana Clara Rolandi*, Cristina Pozo-Gonzalo, Iratxe de Meatzza, Nerea Casado, Maria Forsyth, and David Mecerreyes

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CIDETEC Basque Research and Technology Alliance (BRTA), 20014 Donostia- San Sebastian, Spain

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Affiliation (Institution/organization name, Country)

Abstract:

Poly(vinylidene fluoride) (PVDF) is the most common binder for cathode electrodes in lithium-ion batteries. However, PVDF is a fluorinated compound and requires toxic N-methyl-2-pyrrolidone (NMP) as a solvent during the slurry preparation, making the electrode fabrication process environmentally unfriendly. In this study, we propose the use of carrageenan biopolymers as a sustainable source of water-processable binders for high-voltage NMC811 cathodes. Three types of carrageenan (Carr) biopolymers were investigated, with one, two, or three sulfonate groups (SO₃⁻), namely, kappa, iota, and lambda carrageenans, respectively. In addition to the nature of carrageenans, this article also reports the optimization of the cathode formulations, which were prepared by using between 5 wt% of the binder to a lower amount of 2 wt %. Processing of the aqueous slurries and the nature of the binder, in terms of the morphology and electrochemical performance of the electrodes, were also investigated. The Carr binder with 3SO₃⁻ groups (3SO₃⁻ Carr) exhibited the highest discharge capacities, delivering 133.1 mAh g⁻¹ at 3C and 105.0 mAh g⁻¹ at 5C, which was similar to the organic-based PVDF electrode (136.1 and 108.7 mAh g⁻¹, respectively). Furthermore, 3SO₃⁻ Carr reached an outstanding capacity retention of 91% after 90 cycles at 0.5C, which was attributed to a homogeneous NMC811 and a conductive carbon particle dispersion, superior adhesion strength to the current collector (17.3 ± 0.7 N m⁻¹ vs 0.3 ± 0.1 N m⁻¹ for PVDF), and reduced charge-transfer resistance. Postmortem analysis unveiled good preservation of the NMC811 particles, while the 1SO₃⁻ Carr and 2SO₃⁻ Carr electrodes showed damaged morphologies.

Biography:

Ana Clara obtained her degree in Materials Engineering (2020) at the Nacional University of Mar del Plata (Buenos Aires, Argentina). During her thesis, she studied green corrosion inhibitors for construction steel, at the Applied Electrochemistry division of the Research Institute for Materials Science and Technology (Argentina). As part of the StorEnergy project, Ana Clara is undertaking a cotutelle project between POLYMAT (Spain), CIDETEC (Spain) and Deakin University (Australia). The project focuses on synthesising and screening water-soluble polymeric binders for Li-ion batteries.

Natural Coaxial Plant Tips Reach Ultrahigh Toughness and Sharpness.

Binodhya Wijerathne^{1*}, Ting Liao², Ken Ostrikov¹ and Ziqi Sun¹

¹Centre for Materials Science, Queensland University of Technology, 2 George Street, Brisbane, QLD 4000, Australia

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Abstract:

Materials with extraordinarily superior qualities are in fast development owing to inspiration drawn from natural structures and mechanisms. This basis is known as bioinspiration. In this work, an ultra-tough and sharp tip structure of natural *Agave striata* leaves is observed, which presents 15-fold higher hardness, 10-fold higher Young's modulus, and approximately 100-fold higher compressive strength than the natural balsa wood. It is noteworthy that the mechanical properties of these natural *Agave striata* leaf tips outperform those of reported wood and wood-like materials as determined in Ashby plots. We show that the exceptional compression strength, stiffness, and toughness are derived from a tightly packed longitudinal bundle of microfibrils composed of coaxially stacked alternative hard lignin and viscoelastic bio-polymer layers with a thickness of around 300 nm, where the lignin layers provide mechanical strength and stiffness while the filled biopolymer layers accommodate deformation and dissipate damage energy. The combination of stiffness and toughness supports the natural tip with appealing sharpness, which may inspire the creation of simple penetrating and retracting micro-needles. The discovery of the exceptional *Agave striata* leaf-tip structure-mechanical property relationship provides a new principle in the manufacturing of strong and tough fibril composites and ultra-sharp micro-needles, as well as a novel model for the creation of bioinspired innovative materials.

Biography:

Binodhya Wijerathne is currently a Ph.D. candidate under the supervision of Professor Ziqi Sun at the Queensland University of Technology, Australia. She received her Master of Philosophy from the same group in 2021. Before her postgraduate studies, she finished her Bachelor of Science Honours in 2016 from the University of Sri Jayewardenepura, Sri Lanka. Her research interests are bioinspired nanomaterials for sustainable environmental technologies.



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