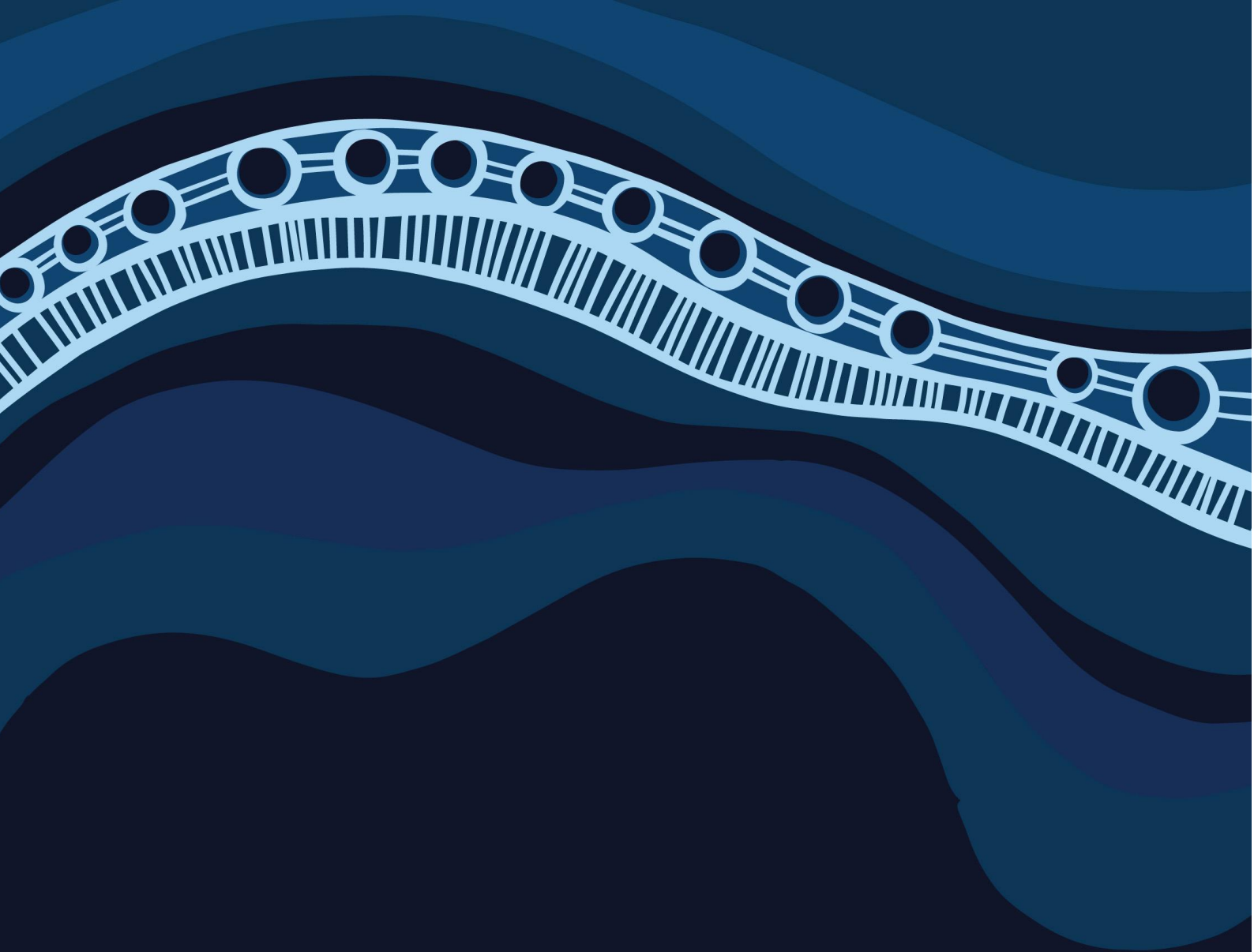




2024 International Symposium on Advanced Materials & Sustainable Technology

11-13 December 2024

Hobart, Australia



ACKNOWLEDGEMENT OF COUNTRY

In recognition of the deep history and culture of this Island, we would like to acknowledge the Muwinina people, the traditional owners of the Land upon which we gather. We acknowledge and pay our respects to all Tasmanian Aboriginal Communities; all of whom have survived invasion and dispossession, and continue to maintain their identity and culture.

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2024 INTERNATIONAL SYMPOSIUM ON ADVANCED MATERIALS & SUSTAINABLE TECHNOLOGY

December 11 - 13, Hobart, Australia

Welcome to AM&ST24

Welcome to the 2024 International Symposium on Advanced Materials & Sustainable Technology (AM&ST24). Following three successful symposiums (AM&ST18 in Brisbane, AM&ST21 in Gold Coast, and AM&ST22 in Cairns), this year's symposium will convene in Hobart, Tasmania, Australia—a city renowned for its carbon-negative status—at the Hobart Convention & Exhibition Centre from December 11 to 13, 2024.

AM&ST24 is an international platform that fosters discussions and builds partnerships across disciplines and borders by bringing together leading scientists, engineers, and industry leaders from around the globe. Our focus is on the latest advancements in advanced materials with the aim of driving forward sustainable technological solutions. The symposium will also address various technological aspects of sustainable energy ecosystems and explore processes that improve energy efficiency while reducing carbon dioxide and other greenhouse gas emissions.

We are proud to welcome an esteemed lineup of leading experts, early career researchers, and students who will share their latest research through the two-day program. As the first post-COVID AM&ST, this international symposium has attracted participants from around the world, including Australia, New Zealand, China, Japan, Singapore, USA and many other countries.

Throughout AM&ST24, you will have the opportunity to connect with colleagues, participate in in-depth discussions on cutting-edge topics, and gain insights from a diverse array of presentations and workshops. We look forward to an engaging and productive conference and hope that your time in Hobart will be both rewarding and memorable. Thank you for being a part of this great event.

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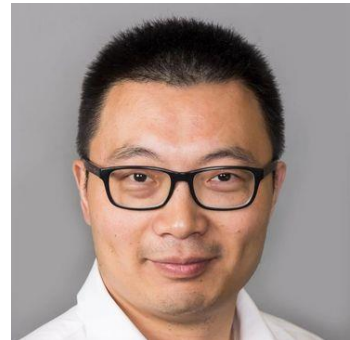
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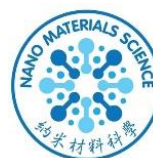
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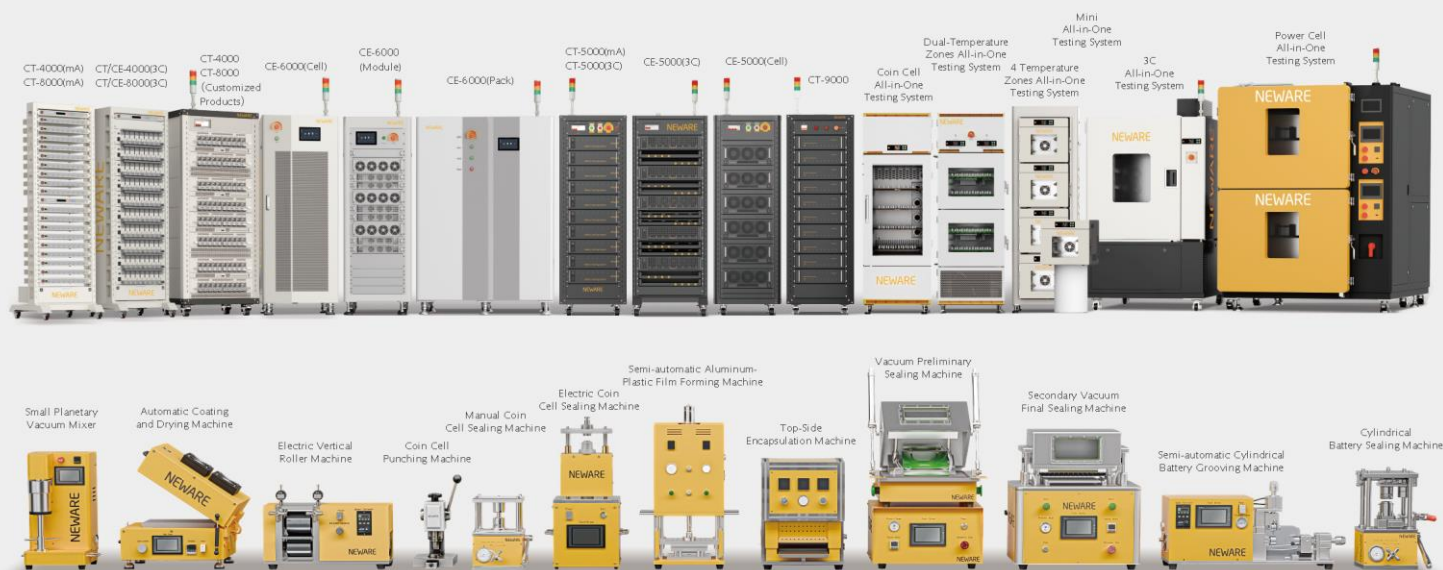
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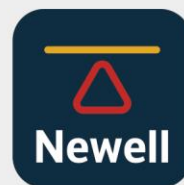
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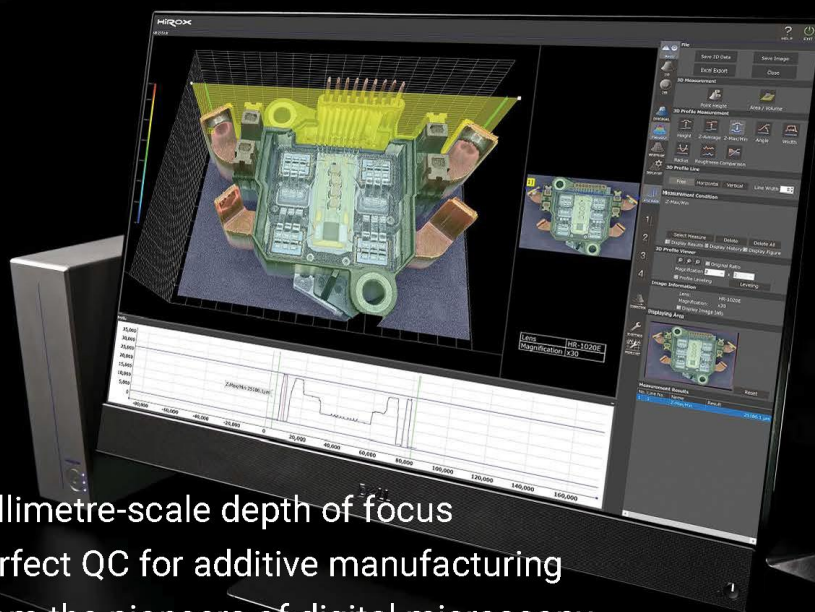
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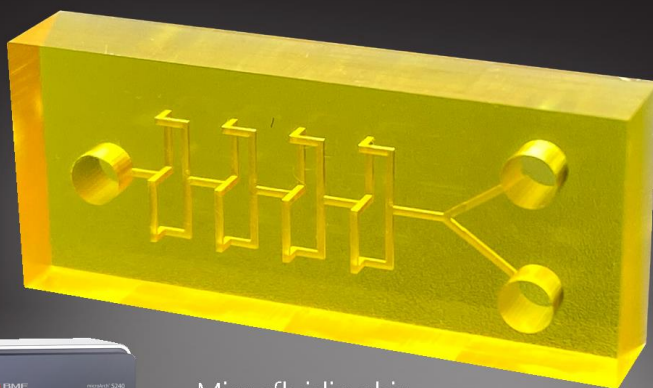
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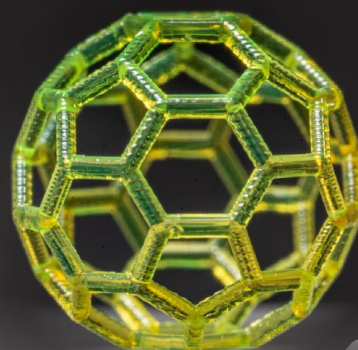
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- CiteScore **17.8**, ranks in Q1 of 3 disciplines in Scopus.
- IF **12.6**, ranks in Q1 of 2 disciplines in the JCR:
 - **37/438**, Materials Science, Multidisciplinary
 - **17/140**, Nanoscience & Nanotechnology



BRIEF

Energy Lab is an open-access journal that covers all disciplines related to energy, publishing cutting-edge scientific and technological achievements in the field of energy science and engineering. Topics include, but are not limited to, **fuel cells, hydrogen energy, secondary batteries, supercapacitors, solar cells, artificial photosynthesis, carbon dioxide conversion technologies, thermoelectric materials, and photothermal materials.**

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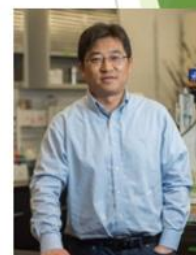
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doi: [10.54227/elab.20230011](https://doi.org/10.54227/elab.20230011)

Xiaoming Xu^{1,2}, Yuanming Zhang^{1,2}, Yong Chen¹, Changhao Liu^{1,2}, Yang Li^{1,2}, Zhonghua Li^{1,2}, Zhetong Yang^{1,2}, Zhaozhong Li^{1,2}, Zhiqiang Zou^{1,2}

A perspective on sulfur-equivalent cathode materials for lithium-sulfur batteries

doi: [10.54227/elab.20220003](https://doi.org/10.54227/elab.20220003)

Huailin Ye¹, Yanguang Li^{1,2,3,4}

Green organic conversion with H₂O₂: challenges and opportunities

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Developments and challenges of catalytic materials for green hydrogen production

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Xiao Liang^{1,5}, Qianqian Wu^{1,5}, Qianqian Liu^{1,2}, Lina Wang¹, Mingcheng Zhang¹, Ke Sun¹, Yucheng Shen¹, Hui Chen^{1,4,5}, Xiaoxin Zou^{1,4,5}

A perspective on the critical design criteria for anode-free metal batteries

doi: [10.54227/elab.20220015](https://doi.org/10.54227/elab.20220015)

Kai Ding¹, Mingyang Zhong¹, Xiaoyuan Zeng¹, Shouyi Yuan¹, Yonggang Wang¹

High safety and fast-charging lithium-ion batteries: a review

doi: [10.54227/elab.20220011](https://doi.org/10.54227/elab.20220011)

Yi Yang^{1,2}, Lei Xu^{1,2}, Chong Yan^{1,2}, Jiaqi Huang^{1,2}, Qiang Zhang¹

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REVIEW ARTICLE

Developments and challenges of catalytic materials for green hydrogen production

Xiao Liang^{1,5}, Qianqian Wu^{1,5}, Qianqian Liu^{1,2}, Lina Wang¹, Mingcheng Zhang¹, Ke Sun¹, Yucheng Shen¹, Hui Chen^{1,4,5} and Xiaoxin Zou^{1,4,5}

Water splitting coupled to renewable power systems is an attractive way to generate green hydrogen and achieve zero carbon emissions, and represents a strategic technology to meet the high demand of carbon-neutral development. Catalysts essentially determine the efficiency and cost of water splitting technologies, and are a class of key materials for green hydrogen production. In this review, we summarize the catalyst developments for the mainstream green hydrogen production technologies, including water electrolysis, water photo-splitting, and photoelectrocatalytic water splitting. We first present basic catalytic mechanisms of these water splitting pathways, as well as emphasize their current research status and challenges for practical application. We subsequently introduce the recent progress in representative catalysts and design strategies toward these photoelectrocatalytic technologies, paying particular attention to water electrolysis, including alkaline water electrolyzer (AWE), proton exchange membrane water electrolyzer (PEMWE), anion exchange membrane water electrolyzer (AEMWE), and solid oxide electrolysis cell (SOEC). Finally, we propose future prospects to develop more desirable catalysts for green hydrogen production at a large scale.



The transformation of current fossil fuel-dominated energy structure to a low-carbon clean one has become a global consensus and mission. Hydrogen is widely viewed as the core of future energy structure, due to its high energy density and zero emissions as energy carrier. It is expected to play a great role in decarbonization of hard-to-abate sectors such as industrial, transportation, chemical, electricity and domestic industries.^[1-3] However, hydrogen for industrial applications is mainly produced by reforming fossil energy (e.g., natural gas reforming) and requiring industrial production (e.g., Haber-Bosch process).^[4] The two pathways benefit from the relatively mature technology and low cost, which have held a dominant status in H₂ in the current hydrogen production systems (also known as grey hydrogen). These pathways not only consume a large amount of non-renewable energy (e.g., coal, oil, natural gas), but also generate high carbon emissions, which are opposite to the conception of green hydrogen.

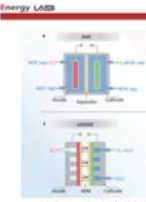


Fig. 1. Schematic diagram of water electrolysis pathways (AWE, PEMWE, AEMWE, and SOEC).

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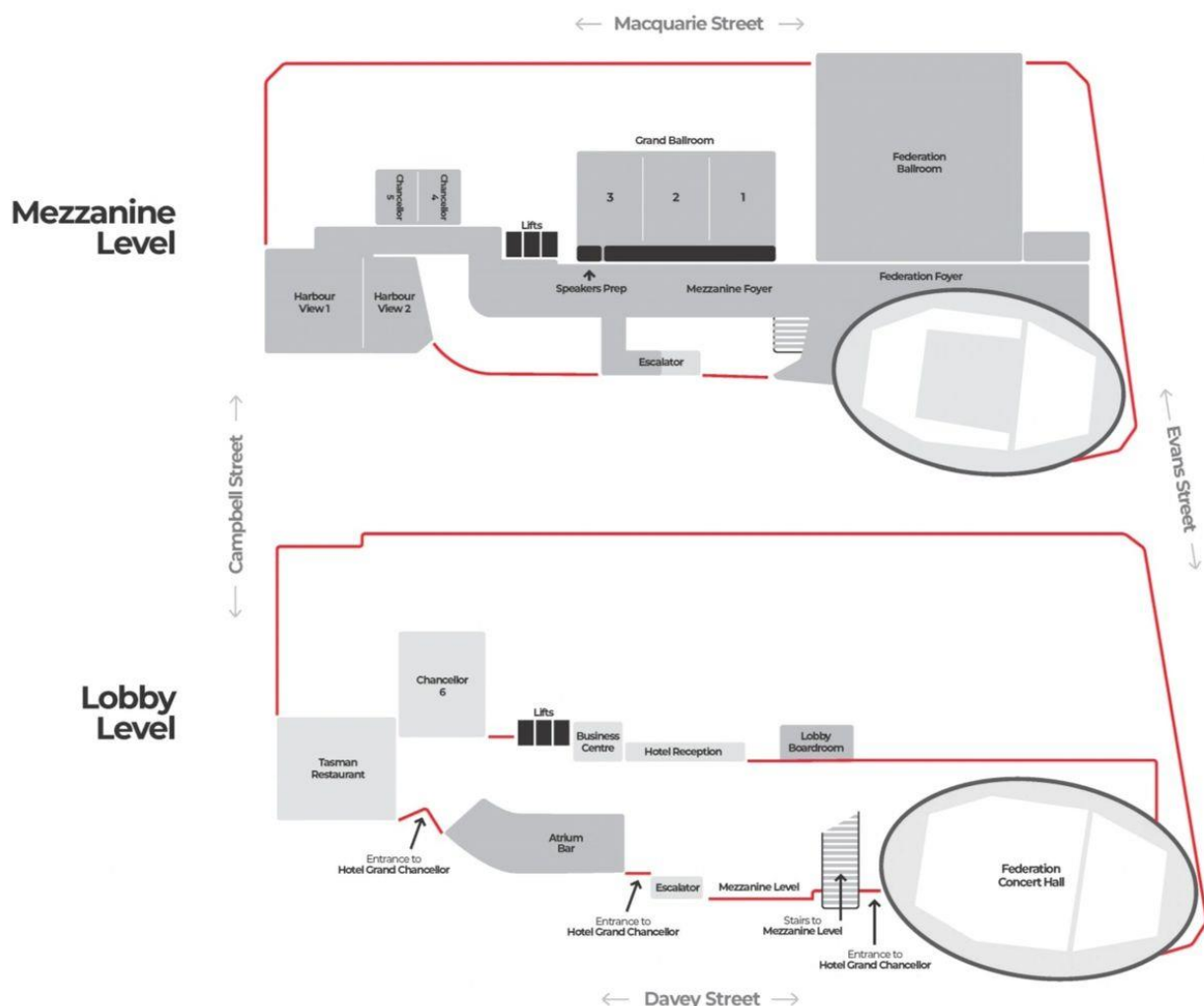
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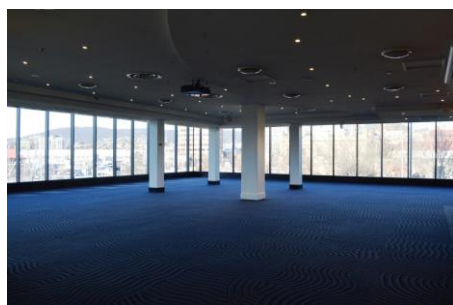


Registration Desk

The Symposium registration desk will be open at the following times:

Wednesday	11 December 2024	14:00-19:00	Mezzanine Foyer, Mezzanine Level
Thursday	12 December 2024	08:30-17:00	Mezzanine Foyer, Mezzanine Level
Friday	13 December 2024	08:30-12:00	Mezzanine Foyer, Mezzanine Level

Social Functions



Welcome Reception

Date: **Wednesday 11 December 2024**

Time: 17:30-19:00

Venue: Harbour View Room One, HCEC



Banquet Dinner

Date: **Thursday 12 December 2024**

Time: 19:00-21:00

Venue: Grand Ballroom, HCEC



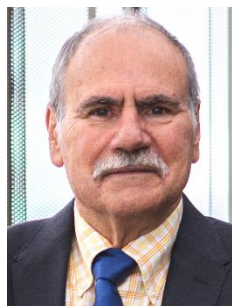
Invited Speaker Dinner

Date: **Friday 13 December 2024**

Time: 19:00-21:00

Venue: Asian Gourmet on the Pier, Elizabeth Street
Pier, Franklin Wharf, Hobart

Plenary Speakers



Professor Michel Armand, CIC energigUNE

Prof. Dr. Michel Armand earned his Ph.D from Université Joseph Fourier in Grenoble. in 1978. He was Director for Research at CNRS, France since 1989 and Professor at U. Montreal (1995–2004). He has pioneered the use of intercalation electrodes (1972), introduced polymer electrolytes (1978), new salts based on delocalized anions, FSI, TFSI, (1986), organic electrode materials (1996) and the carbon coating for LiFePO_4 (1998). He joined CIC Energigune in 2013, and present activities include new solvating polymers for lithium and sodium, new salts and new organic and inorganic electrode materials; Michel Armand has > 500 publications, a H factor of 106; his work has been quoted > 95000 times.



Professor Christopher Barner-Kowollik, Queensland University of Technology

Christopher's research fuses physical and organic chemistry, focussing on the concept of wavelength resolved precision photochemistry. His team introduced the modern-day version of photochemical action plots and a taxonomy for two-colour photochemical processes for materials design termed synergistic, cooperative, antagonistic and orthogonal reaction modes. A graduate of Göttingen University, Christopher joined UNSW rising to lead the Centre for Advanced Macromolecular Design as one of its directors. He returned to Germany to the Karlsruhe Institute of Technology, establishing a German Research Council Centre of Excellence. His research achievements have been recognised by an array of awards including the Centenary Prize of the Royal Society of Chemistry, the Belgian Polymer Medal, the United Kingdom Macro Medal as well as national awards by the Royal Australian Chemical Institute (HG Smith Medal), the Royal Society of New South Wales (David Craig Medal), an ARC Professorial Fellowship and a Laureate Fellowship. He is a Fellow of the Australian Academy of Science, the Royal Society of Chemistry and the Royal Australian Chemical Institute.



Professor Vicki Chen, University of Technology Sydney

Professor Vicki Chen is currently the Provost and Senior Vice-President of the University of Technology Sydney (UTS). Professor Chen graduated with a Bachelor of Science in Chemical Engineering from the Massachusetts Institute of Technology (MIT) and a Ph.D. in Chemical Engineering from the University of Minnesota. She has over twenty-five years research experience in the areas of membrane separation, gas separation, biocatalytic systems, nanomaterials, and water treatment. In the area of carbon capture, she was involved in membrane projects with the Cooperative Research Centre for Greenhouse Gas Technologies (CO2CRC) and Coal Innovation NSW. Prior to joining UTS in 2022, Professor Chen was the Executive Dean of the Faculty of Engineering, Architecture, and IT at the University of Queensland (UQ). Previously, she was a professor in the School of Chemical Engineering at the UNSW Sydney before taking on the substantive Head of School position (2014 – 2018) and was the Director of the UNESCO Centre for Membrane Science and Technology at UNSW (2006 – 2014). Professor Chen is currently on the editorial board for the Journal of Membrane Science and editorial advisory board of Macromolecules and was formerly on the editorial board for the Desalination Journal. Professor Chen is a Fellow of the Australian Academy of Technology and Engineering (ATSE) and a founding board member of the Membrane Society of Australasia.



Professor Hong-jun Gao, Institute of Physics, Chinese Academy of Sciences

Prof. Hong-jun Gao obtained his Ph.D. from Peking University in 1994. He is now a Group Leader in Institute of Physics, an Academician of the Chinese Academy of Sciences (CAS), and an Academician of the Developing-country Academy of Sciences (TWAS). He has served as the vice president of CAS, and is currently the vice president of China Association for Science and Technology (中国科协). His research interests focus on construction and physical properties of quantum nanostructures and scanning tunneling microscopy/spectroscopy. He has published more than 500 journal publications including many on Science, Nature, Nature series, PRL, JACS, Adv. Mater. He was awarded international Awards including the "Humboldt Research Award", the "OCPA AAA (Robert) Prize", and the "TWAS Prize in Physics", and top-level recognitions in China including "Tan Kah Kee Science Awards on Mathematics and Physics", "Science and Technology Awards of the Ho Leung Ho Lee".



Distinguished Professor Baohua Jia, RMIT

Baohua Jia is a Fellow of Australian Academy of Technological Sciences and Technologies (FTSE), a Future Fellow of Australian Research Council and Founding Director of Centre for Atomaterials and Nanomanufacturing (CAN) at RMIT University, Australia. Before joining RMIT University in 2022, Baohua was a tenured professor at Swinburne University of Technology and Founding Director of Centre for Translational Atomaterials. Professor Jia is a Fellow of Optica (previously known as the Optical Society of America), and a Fellow of the Institute of Materials, Minerals and Mining (FIMMM). Professor Jia's research focuses on the design and optical characterization of novel nanostructures and nanomaterials, fabrication, and efficient conversion and storage of light energy. As a leading Chief Investigator, Professor Jia received a total of more than \$80 million in research funding support. Professor Jia has published more than 300 journal papers with an h-index of 77 (Google Scholar) and developed over 20 invention patents and patent applications, many of which have been commercialized. Based on Professor Jia's outstanding contributions in scientific research, she has won many awards, including the 2021 Veski Fellow, 2017 finalist of the Australian Prime Minister's Science Award, the Vice Chancellor's Industrial Achievement Award in 2011, 2016, and 2018, 2013, Young Science Leader Award, 2012 UNESCO L'Oréal Australia New Zealand Women in Science Award.



Professor Kourosh Kalantar-Zadeh, University of Sydney

Kourosh Kalantar-Zadeh is a Professor and Head of School of Chemical and Biomolecular Engineering at the University of Sydney. He is also one of the Australian Research Council Laureate Fellows of 2018. Kalantar-Zadeh was a professor of Chemical Engineering at UNSW, and prior to that a Professor of Electronic Engineering at RMIT, Australia. Kalantar-Zadeh is involved in research in the fields of analytical chemistry, materials sciences, gastroenterology, electronics and sensors, and has co-authored of >500 highly cited scientific papers. He is a member of the editorial boards of journals including ACS Applied Nano Materials (associate editor), ACS Sensors, Advanced Materials Technologies, Nanoscale, Applied Surface Science and ACS Nano. Kalantar-Zadeh is best known for his works on ingestible sensors, liquid metals and two-dimensional semiconductors. He led his group to the invention of an ingestible chemical sensor: human gas sensing capsule, one of the breakthroughs in the field of medical devices. Kalantar-Zadeh has received several international awards for his scientific contributions including the 2017 IEEE Sensor Council Achievement, 2018 American Chemical Society Advances in Measurement Science Lectureship awards and 2020 Robert Boyle Prize of Royal Society of Chemistry.



Distinguished Professor Yun Liu, Australian National University

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

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



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PLENARY PRESENTATION

The coming (r)evolution in batteries

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The transition to a carbon-free economy will require tens of millions of tons of batteries to be produced in the forthcoming years, to power electric vehicles or, even more demanding in tonnage, to accommodate the fluctuations of renewable energies. Australia has the potential to become a net exporter of green electricity, mainly from photovoltaics.

To improve on the energy density required to enhance the driving range and thus acceptability of EVs, a transition to the use of a metallic lithium electrode is needed. This can only be considered with unconventional electrolytes, and solids seem the most promising. Polymer electrolytes are seen as one safe way of harnessing the repeated plating and dissolution of this ultra-reactive metal, prone to grow into dendrites and creating short circuits.

Poly(ethylene oxide) PEO has been the most studied polymer host in which various salts of low lattice energy can be dissolved, leading to useful ionic conductivity. Not only lithium, but sodium and potassium can be moved in such macromolecular lattice. PEO is however a crystalline polymer, while conductivity occurs mainly in the amorphous phase reached above 65°C. We have been successful recently in modifying the polymer architecture, with a comb structure, into fully amorphous material at room temperature, with improved conductivity. Another problem with polymer electrolytes, similar to liquid solutions, is that, when a salt is dissolved, both anions and cations are mobile; this is deleterious to the operation of the battery with the build-up of concentration gradients and the triggering of dendrite growth. To solve this, poly(salts) in which the anionic part is tethered to a macromolecule, thus immobile have been designed and synthesised. When this polysalt is alloyed with a solvating host, the so-called “single-ion” electrolytes are obtained.

For grid storage, the demand is less on energy density than on extensive lifetime (≥ 10 years) and price. In this respect, sodium batteries offer interesting advantages for several reasons besides the obvious greater abundance of Na (2,75% of earth crust) vs. Li (25 ppm): i) electrode materials devoid of cobalt and nickel can be deployed; ii) the negative electrode current collector, which is mandatorily copper in lithium batteries, can be replaced by far more sustainable aluminium. > 4000 cycles have already been demonstrated in commercial systems with little capacity fading.

Today, solid-state polymer electrolyte lithium metal batteries (SSLMB) are commercial in France and Germany on buses (Blue Solutions & Daimler) and give entire satisfaction. The emphasis is now on reducing the operating temperature from 70°C to RT.

The Precision Photochemistry Paradigm

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Over the last decade our laboratory has employed monochromatic tuneable laser systems to reveal a strong mismatch between the absorptivity of a chromophore and its photochemical reactivity in the vast majority of covalent bond forming as well as bond cleavage reactions. Our data overturns the long-held paradigm that effective photochemical reactions are obtained in situations where there is strong overlap between the absorption spectrum and the emission wavelength under a given set of reaction conditions. However – as we explore herein – the absorption spectrum of a molecule provides only information about singlet excitation and remains largely silent on the accessibility of the critical triplet states, which dictate photochemical reactivity. We propose future avenues of enquiry on how photochemical action plots can be understood and demonstrate how they are of key importance for tailoring photochemical applications in light-driven soft matter materials design – including in advanced light-driven multi-material 3D printing – with never-before-seen precision, exploiting wavelength orthogonal, synergistic, cooperative and antagonistic photochemical reaction modes.

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Horizons for Coordination Polymers: Membrane Separation and Devices

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Since the advent of metal organic framework and coordination framework materials emerged in the last two decades, the chemical and structural architectures available have increased exponentially. The focus has evolved from rigid topology and porosity to flexible frameworks to “soft” glassy and liquid structures enabling new synthesis and processing approaches. These latter materials were outlined by Horike et al. [1] as fourth generation coordination polymers. The span of constructs and architectures for separation, catalysis, and interfacial engineering has consequently developed in the last ten years to exploit not just their own precise topology but unique ability for these materials to scaffold other materials in their matrix. Examples range from membrane materials which provide precise gas and ion separation and enzymatic cascades to more recent work using glassy MOF and COF matrix to constrain phase change of perovskites, optimising their stability and light-emitting performance. The synthesis and processability of these materials through mechanochemistry and melting are also explored to generate new form factors for devices.

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Ordered and tunable Majorana-zero-mode lattice in iron-based superconductors

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Abstract:

Majorana zero-modes (MZMs) are spatially-localized zero-energy fractional quasiparticles with non-Abelian braiding statistics. They are believed to hold great promise for topological quantum computing. Based on our research work on construction and atomic manipulation of novel 2D atomic crystals and the physical properties [1-4], and by using low-temperature and strong-magnetic-field scanning tunneling microscopy/spectroscopy, A clean Majorana zero mode has been firstly observed in a single material platform of high- T_c iron-based superconductor, FeTe_{0.55}Se_{0.45} [5]. The mechanism of two distinct classes of vortices presented in this system was revealed, which directly tied with the presence or absence of zero-bias peak [6]. We further found the Majorana conductance plateau in vortices. Both the extrinsic instrumental convoluted broadening and the intrinsic quasiparticle poisoning can reduce the conductance plateau value, and when extrinsic instrumental broadening is removed by deconvolution, the plateau nearly reaches a $2e^2/h$ quantized value [7]. Most recently, we have successfully achieved the large-scale, highly-ordered and tunable MZM lattice in strained LiFeAs. More than 90% of the vortices are topological and possess the characteristics of isolated MZMs at the vortex center, forming ordered MZM lattice with the density and the geometry tunable by external magnetic field. With decreasing the spacing of neighboring vortices, the MZMs start to couple with each other [8]. This kind of materials combine the advantages of a simple material, high- T_c , large ratio of Δ/E_F and etc. These results show a great potential of MZMs in the application of topological quantum computations in the future.

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Atomaterials for Sustainability

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“Atomaterials” represents materials with at least one dimension on the atomic scale. Their properties depend on the precise configuration of their atoms. It is a new but rapidly developing field. A typical atomaterials is graphene, which is made of carbon atoms. Unlike diamond, in which the carbon atoms form a rigid three-dimensional structure, graphene is made of single layer of carbon atoms, bonded together in a two-dimensional honeycomb lattice. They show exceptional properties due to their atomaterials nature. Using atomaterials, our lab has been working on a range of innovations, at various stages of development, for example: A diurnal cooling film without consuming electricity. This film can cool the environment by up to 15°C without using any electricity. By integrating such a film into a building, the electricity used for air conditioning can be dramatically reduced. This will not only save electricity bills but also reduce greenhouse emissions; Heat-absorbing film, achieving over 97% of energy conversion rate with an ultrathin film arrangement [1-4]. These materials play critical role in improving energy efficiency and providing innovative sustainable solutions for our society.

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Transformation of Chemical Processing by Liquid Metals

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Chemical reactions account for approximately 12% of global greenhouse gas emissions and a significant portion of the world's energy consumption. Many modern chemical processes depend on solid-state catalytic materials across various facilities. These solid catalysts typically have fixed atomic structures that form active sites, which, although effective at lowering reaction energy barriers, often lack the atomic-level flexibility required to maximize efficiency and selectivity in certain processes.

In contrast, liquid metals—metals and alloys that are liquid at or near room temperature—have the ability to rearrange interfacial atom positions in response to surface reactions. This dynamic behavior can be viewed as a form of innate intelligence, where freely moving liquid-state atoms are guided to optimal positions, enhancing catalytic functionality. This flexibility holds the potential to create energy-efficient reaction pathways and enable reactions not feasible in solid-state systems [1-3].

This presentation will discuss an exploration on how liquid metals could improve a variety of chemical reactions, including green hydrogen production, the synthesis of fine chemicals with precise structures, and the breakdown of persistent substances like microplastics and per- and polyfluoroalkyl substances. While the use of liquid metals in chemical reactions is still in its early stages—especially compared to solid surfaces, which have been studied for over 200 years—their potential to harness atomic "intelligence" for driving reactions could revolutionize the future of the chemical industry.

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Chemistry, structure and scale matters in ferroelectric study

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Ferroelectric materials are strong correlated solid-state systems that contain extremely rich chemistry and physics. Introducing external ions in a solid solution can modulate the property of materials to achieve the targeting performance for various applications. This is why the ferroelectric study has been enduring for more than century. The applications of ferroelectrics and its derivatives have been extended to the catalysis for energy and environment, and quantum effect for quantum technology and ultralow-energy consumption devices for big data etc emerging technologies. Nowadays, utilizing start-of-the-art characterization technologies, ones enable uncovering more comprehensive chemical and structural information of materials at different lengths scale. It is often found that the ferroelectric behaviors cannot be defined or well described by a simple, classical ferroelectric concept. The local chemical and structural correlation length/volume become important to be considered. It will become even critical when machine learning and artificial intelligent (AI) are employed for materials design, and when nanoferroelectric materials are studied. In this talk, I will review the original ferroelectric concept, discuss potential chemical and structural issues in ferroelectric study, and explore the solutions to get precise chemistry and structure information for new generation materials design and to develop new ferroelectricity beyond existing ferroelectric materials systems for emerging technologies.

Electrocatalytic Refinery for Production of Fuels and Chemicals

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

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

How Far and How Fast Can Green Hydrogen Fantasy Go?

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“Net Zero” by decarbonising the planet has been a goal that many prescribe or subscribe to around the world. To achieve this, hydrogen has once again been toasted as an energy carrier or [zero-carbon] fuel that would not incur any [“carbon”] emissions, giving rise to green hydrogen in recent times. This presentation aims to provide a brief overview of the history of hydrogen economy, sharing the speaker’s own scientific research, engineering practice, and entrepreneurship in hydrogen as well as methanol and ammonia as his preferred hydrogen carrier, and to outline the challenges and opportunities in the request for green hydrogen.

KEYNOTE PRESENTATION

Nucleation and Dynamics of Nanobubbles in Chemical Environment

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Stability of nanobubbles remains a highly debated topic [1, 2]. Understanding how to generate these nanobubbles and their response to chemical stimuli as gas carriers is essential for their practical applications. This talk covers three parts, bulk nanobubble generation approaches through porous materials[3], and their stability, and applications for cleaning[4]. For small-scale nanobubble nucleation, we used a syringe-based method to nucleate nanobubbles by passing a gas-liquid mixture through nanopores, achieving high concentrations of uniformly dispersed nanobubbles in amino acid solutions [3], enabling them suitable for biomedical applications such as drug delivery and cell culture. mixture of gas and solutions were passed through a nanopore using syringes. For large scale, we immersed carbon and zeolite molecular sieves in water to generate nanobubbles without any extra energy input and can generate oxygen or nitrogen nanobubbles. With this protocol, we successfully produced oxygen and nitrogen nanobubbles as indicated by the levels of dissolved oxygen. This oversaturated water with specific dissolved gases can be used for improving outdoor water qualities to suppress anaerobic or aerobic microbes. For bubble stability, we designed an experiment to assess how nanobubbles respond to chemical stimuli. We hypothesized that depleting oxygen in the bulk liquids can lead to the death of surface air nanobubbles. However, the adding of oxygen scavenger in bulk did not kill the surface nanobubbles. Instead, the surface nanobubbles are super stable, subjected to minor changes in height and contact angles. Oxygen scavenger consumes dissolved oxygen, leading to increasing dissolved nitrogen, super charging the pinned surface nanobubbles. Finally, we explored nanobubbles for cleaning surface contaminated oils without any detergents, offering a low-cost and efficient cleaning solution.

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Engineering Nanostructured Materials via 3D Printing with Fully Recyclable Resins

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Abstract: Currently, there are no straightforward methods to 3D print materials with nanoscale control over morphological and functional properties. In this talk, a novel approach for the fabrication of materials with controlled nanoscale morphologies using a rapid and commercially available Digital Light Processing 3D printing technique will be presented. The approach uses a controlled/living radical polymerization technique, more specifically, reversible addition-fragmentation chain-transfer (RAFT) polymerization, to control the topologies of the polymers.¹⁻² In this talk, we report a rapid visible light mediated polymerization process and applied it to a 3D printing system.³ Following the optimization of the resin formulation, a variety of 3D printing conditions will be presented to prepare functional materials.⁴ The mechanical properties of these 3D printed materials were investigated under different conditions, showing that the control of the polymer structure can affect the performance of these materials.⁵ Furthermore, the polymer networks were able to be reactivated after the initial 3D printing process, which allowed the post functionalization of the printed materials via secondary photopolymerization processes, enabling to introduce information.⁶ Finally, by controlling the polymer architecture, we were able to precisely control the nanostructure of these 3D printed materials via a polymerization induced microphase separation.⁷ The effect of nanostructure on 3D printed material properties will be discussed as well as their potential applications in drug delivery and energy storage, such as their use as solid polymer electrolytes for supercapacitor application. Finally, we will discuss a new approach for the recovery of resin after 3D printing enabling to recycle these 3D printed materials.

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Plasma-assisted Catalysis for Ammonia Production and Carbon Dioxide Methanation

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Applying atmospheric-pressure plasmas to catalytic processes provides several advantages over thermal catalysis, including operation at ambient conditions and small scale, using electrical power, and rapid turn-on and turn-off, all of which increase compatibility with renewable energy sources [1]. Plasma is viewed as a potential contributor to the electrification of the chemical industry, which will be required to meet greenhouse gas emission reduction targets [2]. Applications being investigated include CO₂ hydrogenation, dry reforming of methane and ammonia production.

The interactions between the plasma and catalyst are far more complex than between the gas and catalyst in thermal catalysis. The chemical species present in the plasma include vibrationally and electronically excited molecules, atoms and ions, as well as the input ground-state molecules, so many more reaction paths are available. Further, the presence of the catalyst and support structure affects the plasma properties.

Ammonia production from nitrogen and hydrogen ($\text{N}_2 + 3\text{H}_2 \rightarrow 2\text{NH}_3$) is one of the most intensely studied reactions. Some studies (e.g. [3]) proposed that vibrational excitation of the nitrogen molecules in the plasma provided an energetically favourable reaction pathway. However, recent experimental and modelling results (e.g., [4]) have shown that the reaction mainly proceeds via the dissociation of nitrogen molecules in the plasma, severely limiting the energy efficiency of the plasma process to well below that of the benchmark thermal catalytic process (the Haber–Bosch process).

In contrast, plasma-assisted CO₂ methanation ($\text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{H}_2\text{O}$) exhibits competitive methane yield, selectivity and energy efficiency to the thermal catalytic process (the Sabatier process) while operating at a much lower temperature [5]. The plasma-assisted process shows significant potential for application to the production of green methane from biogas.

The physics, chemistry and materials science relevant to the two processes will be compared, and the potential for industrial application of plasma catalysis will be considered.

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Interface Engineering for Hydrogen Evolution Reaction

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

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

Nanodiamond as a biocompatible platform for bioimaging and efficient drug delivery

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Nanodiamond (ND) has been showing great potential in bio/medical applications for bio imaging and drug delivery owing to its superb spectroscopic properties. The fluorescence properties of ND are determined by defects and admixtures in the crystal lattice or on the surfaces. This provides a stable and non-photobleaching fluorescence for imaging. ND's surface can be functionalized to form complexes with biomolecules of interest. ND has been proven to be excellent biocompatible with various cancer and non-cancer cells [1]. These render ND the possibilities of drug conjugation and delivery. Combining these advantages, image-guided drug delivery systems for preclinical applications can be realized.

Upon interaction with cells, ND penetrates inside the cytoplasm of the cells. The possible internalization pathways affect the possibility of delivering drug molecules to the targeted sites of the cancer cells. The applications can require the relinquishing ND-drug conjugate via blood flow, where interaction with immune cells may occur; and the interaction of ND with blood cells, the influence of the ND on the cell oxygenation capabilities are also important factors. We found, ND was engulfed by macrophages via clathrin-dependent endocytosis pathway and is observed mainly encapsulated in the lysosome inside the cytoplasm. This can particularly explain the inertness of ND in interaction with the intercellular structures, as the limited side-effects provoked by ND in its bio applications, which gives the chance of ND as a biocompatible vehicle for drug delivery.

ND can be a convenient platform for bio applications; however, proper conditions are extremely important. The understanding of the engulfment mechanism allows control the ND-containing complex (ND-based conjugate with drugs, etc.) tracing in the tissue, as well as the interaction with the macrophage and target cells. Various examples of imaging and drug delivery that have been realized in the cellular models [2]. However conventional 2D cell culture model does not represent 3D structural of tissues and tumors, the 2D cellular models offer poor access to the efficiency of drug delivery. To address this, we developed a 3D multicellular tumor spheroid (MCTS) of Human alveolar basal epithelial cell (A549) cellular model to demonstrate the possibility of using ND for drug delivery and to evaluate the efficacy of the drug conjugate of ND-Drug in cancer therapy.

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Atomic-scale Manipulation of Single-Polaron in a Two-Dimensional Semiconductor

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Polaron is a fundamental physical phenomenon associated with the behavior of charges in insulators or semiconductors. Different from metal where the excess charge can flow as current and easily be compensated, insulators or semiconductors usually have charges stuck inside. Excess charge (electron or hole) trapped by self-induced lattice distortion due to electron-phonon coupling interaction (EPI) is named as polaron. Polaron has significant influences on the properties of semiconducting materials, such as lattice reconstructions, carrier mobility, surface adsorption and catalysis, ferromagnetic transition, superconductivity, and other many-body correlation states. The investigations and applications of polaron have been developed as an emerging field in nanotechnology, named as ‘Polaronics’. However, atomic-scale creation and manipulation of single-polarons in real space have still not been achieved so far, which precludes the atomistic understanding of the properties of polarons as well as their applications.

Herein, using scanning tunneling microscopy, we succeeded to create single polarons in a monolayer two-dimensional (2D) semiconductor, transition metal dichloride CoCl₂. Through applying a voltage pulse, we can inject an electron into the monolayer CoCl₂ and create two types of electron polarons. First principles calculations indicate that they can be described as spin-polarized electrons bonded to lattice distortions centered at either atop site or hollow site of the surface, respectively. Remarkably, a series of manipulation progresses — from creation, erasure, to transition — can be accurately implemented on individual polarons. Our results pave the way to understand the physics of polaron at atomic level, and the easy control of single polarons in 2D semiconductor may open the door to 2D polaronics including the data storage.

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Developing Safe and Reliable Battery Technologies

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This presentation will provide an overview of our ARC Research Hub on Safe and Reliable Energy Storage and Conversion Technologies. Established in 2021 through an ARC grant to Deakin University, alongside five partner universities and ten industry partners, this National Research Hub aims to address critical challenges in battery safety and reliability. As batteries play an increasingly important role in our lives, from powering everyday electronic devices to electric vehicles, issues related to safety and the circular economy have become major concerns affecting both society and the environment.

The Hub's research teams are collaborating with industry partners to tackle these challenges. For example, Deakin University is working with LiS Energy Ltd on developing safe, solid-state batteries that eliminate the need for flammable organic liquid electrolytes. The University of Adelaide is focusing on water-based zinc batteries for enhanced safety, while the University of Queensland is advancing flow batteries for large-scale, safe energy storage. Meanwhile, the University of Sydney, in partnership with Hazer Group, is developing new carbon materials to support a circular economy.

The Hub's research has a direct impact on the safe application of battery technologies in our communities. Notably, the University of Wollongong team has collaborated with Shoalhaven Water, NSW, to implement battery systems as reliable power sources for water facilities during periods of electricity grid instability and failure. The outstanding research from this ARC Hub is making a meaningful difference to both industry and society.

Engineering Cathode Layers for PEM Fuel Cells

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Proton exchange membrane fuel cells (PEMFC) are among the most promising clean power generators for tomorrow's energy needs as these power generators have high electrochemical conversion efficiency and producing clean water as waste. These cells operate at a relative safe and low temperature of 80 °C hence making these PEMFC highly suitable for mobile and transportation applications. Furthermore, it has other advantages such as no moving parts, solid electrolyte, silent operations and no harmful emission. Currently, durability and robustness 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 PEMFC operations. For example, we have fabricated hybrid 1D carbon nanocomposites mounted on carbon template structures which clearly demonstrated higher activity and robustness over the standard carbon black (VXC-72R). We can further integrate other unique allotropes of 1D/2D hybrids where excellent energy conversion and robust properties have been obtained. We will further show that there may be other reasons behind Sulphur-based degradation processes which is not well understood at the moment. This may allow us to fabricate new carbon support structures to create next generation of robust PEMFCs. 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.

ABSTRACTS

Challenges and Opportunities for Green Hydrogen Production and Utilisation in Water Electrolysers and Fuel Cells

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

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

Liquid metal colloids – A unique type of chemistry is coming into focus

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Liquid metals are an emerging class of compounds that are liquid close to room temperature yet exhibit metallic conductivity [1]. Liquid metals have found application in the design of flexible and reconfigurable electronics and more recently emerged as a platform for the synthesis of nanostructures [2] as well as a unique class of catalysts that is extraordinarily resilient towards deactivation [3]. In comparison to other liquids such as covalent solvents and ionic liquids, comparatively little is known about the chemistry that occurs inside molten metals. This talk covers the emerging picture of liquid metal chemistry and will report our most recent results for solid-metal-in-liquid-metal colloidal systems. In a second part of the talk, our recent results in the area of CO₂ reduction to graphene and NH₃ synthesis will be covered.[4]

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Single atom catalyst for water purification

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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.

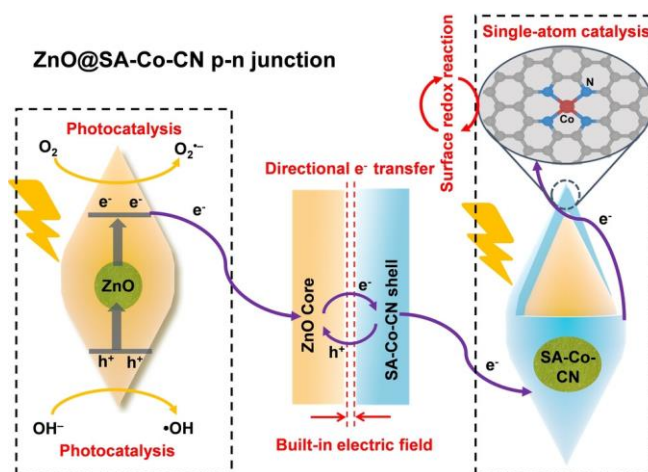


Figure 1 Mechanisms of SACs in persulfate activation under solar light irradiation

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Surface and Interface Enhanced Properties in 2D Monolayers and Heterostructures

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The quest for sustainable technologies has led to a surge in research on two-dimensional (2D) monolayers and heterostructures, which are envisioned as key materials for building a green future. These atomically thin materials offer unprecedented opportunities for material innovation due to their unique electronic, optical, and magnetic properties. The integration of 2D magnetic materials with other layers has opened new avenues for enhancing performance and inducing novel phenomena, which are crucial for energy-efficient computing, data storage, and spintronics. This presentation will highlight how intralayer and interlayer interactions can be harnessed to manipulate properties such as magnetism, ferroelectricity, and optical responses, paving the way for eco-friendly electronic devices. Firstly, I will talk about the chemical reactions happened on surfaces and the corresponding activation enhanced by the adsorption of the precursor molecules at specific site. Second, the coupling of multiple order parameters in 2D monolayers and bilayers will be discussed. The coupling allows for the manipulation of properties such as spin polarization, electronic band topology, and valley polarization. This multifunctionality offers new possibilities for designing hybrid devices that leverage multiple properties simultaneously, leading to efficient and versatile electronic devices. Thirdly, the high-throughput screening and machine learning classification of van der Waals dielectrics for 2D nanoelectronics will be discussed. These studies have accelerated the discovery of new materials with tailored properties, enabling the rapid progress from theoretical prediction to practical application.

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2D Frustrated Materials with Exotic Electronic Structures

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Quantum destructive interference (QDI) in two-dimensional (2D) geometrically frustrated systems can give rise to flat bands (FBs) in electronic energy dispersion relations. Such degenerate manifold of single-particle states has attracted great attention not only in non-trivial topological states induced by spin-orbit coupling (SOC), but also in exploring strongly correlated electron phenomena due to the significantly enhanced electron-electron interaction in FBs. However, the scarcity of pure 2D frustrated lattice in natural materials makes FBs hard to be identified, let alone the FB relating electronic properties. In this talk, I will introduce the strategy to design and fabricate low-dimensional frustrated lattices, including kagome, Lieb, and colouring triangle lattices, which host FB electronic structures [1-7]. The FBs possess suppressed bandwidth with high density of states and exotic characteristics, which are directly confirmed by scanning tunneling microscopy, angle-resolved photoemission spectroscopy, and the first-principles calculation. The 2D frustrated materials with exotic electronic structures show a great potential in energy conversion and storage.

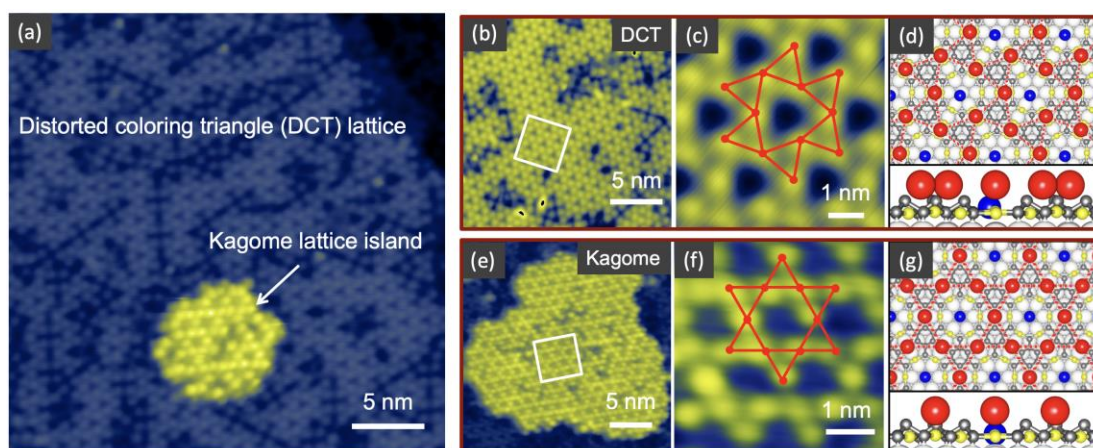


Figure. STM images of two frustrated kagome and distorted colouring triangle lattices with flat bands

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Imaging topological polar structures in marginally twisted 2D semiconductors

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Moiré superlattices that arise in van der Waals heterostructures due to twist, lattice mismatch and strain offer the potential to design new metamaterials that host properties that are not present in the individual layers of the materials themselves. Ferroelectricity for example, arises due to broken inversion symmetry in twisted and strained bilayers of 2D semiconductors with ferroelectric domains of alternating out-of-plane polarization [1,2]. The ability to detect whether the ferroelectricity in marginally twisted 2D semiconductors arises due to twist or strain remains elusive. Inversion symmetry breaking also gives rise to an in-plane component of polarisation along the domain walls that is predicted to form a network of topologically non-trivial merons (half-skyrmions) that are Bloch type for twist and Néel type for strained systems [3].

In this talk I will discuss the use of piezoresponse force microscopy (PFM) to probe the in-plane polarisation component in marginally twisted bilayer WSe₂. Varying the tip direction with respect to the orientation of the domain walls allows the polarization components and topological polar nanostructures in marginally twisted bilayer WSe₂ to be spatially resolved. This provides experimental proof for the existence of topologically non-trivial meron/antimeron structures, with the observation of both Bloch-type and Néel-type merons, allowing differentiation between moiré superlattices formed due to twist or heterogeneous strain. This first demonstration of non-trivial real-space topology in a twisted van der Waals heterostructure will open new pathways for exploring the connection between twist and topology in engineered nano-devices.

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Flexible Thin Film Solar Cells: Opportunities and Challenges

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Solar energy, the most abundant source of renewable energy, is at the forefront of the global transition to net-zero emissions in the 21st century. Unlike the conventional manufacturing processes used for silicon solar cells, advancements in high-volume, low-cost roll-to-roll (R2R) printing techniques have transformed thin-film solar cell production. This process involves the continuous deposition of solar cell components onto flexible substrates using scalable coating methods, enabling the production of lightweight, rollable, and highly efficient solar cells while significantly reducing costs. The innovative design of these solar panels also results in high specific power (power-to-weight ratio), making them particularly attractive for emerging applications, including space exploration, drones, vehicle-integrated photovoltaics (VIPV), and building-integrated photovoltaics (BIPV).

This presentation will provide an overview of the latest developments in R2R printing technologies. A major focus has been on bridging the efficiency gap between devices fabricated using lab-scale spin coating and those produced with scalable deposition methods. Substantial efforts have been directed toward achieving reliable, pinhole-free, and uniform films via the R2R deposition process. Our work has demonstrated the highest power conversion efficiency (PCE) for fully vacuum-free R2R-fabricated solar modules [1]. Additionally, a deeper understanding of the thin-film formation process has shed light on how this influences film quality. By identifying key challenges and optimizing deposition techniques, these innovations are poised to make a significant impact in the broader solar energy community.

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The Applications of Grazing Incidence Wide Angle X-ray Scattering

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In the first part of this talk, the status of Shanghai Synchrotron Facility (SSRF) will be introduced. There are 34 beamlines with 46 end stations in operation currently, which offer great opportunities in various fields. In the second part, the synchrotron based Grazing Incidence Wide Angle X-ray Scattering (GIWAXS) will be introduced. As an example, the applications of GIWAXS in the study of organ-inorganic hybrid lead halide perovskite will be present. At the end, GIWAXS with micro beam will be shown to bring new opportunities in the study of thin films. First of all, micro beam will reduce significantly the footprint effects as shown in Figure 1(b). In addition, scanning μ -GIWAXS can be employed to map thin films, providing spatially resolved microstructural information.

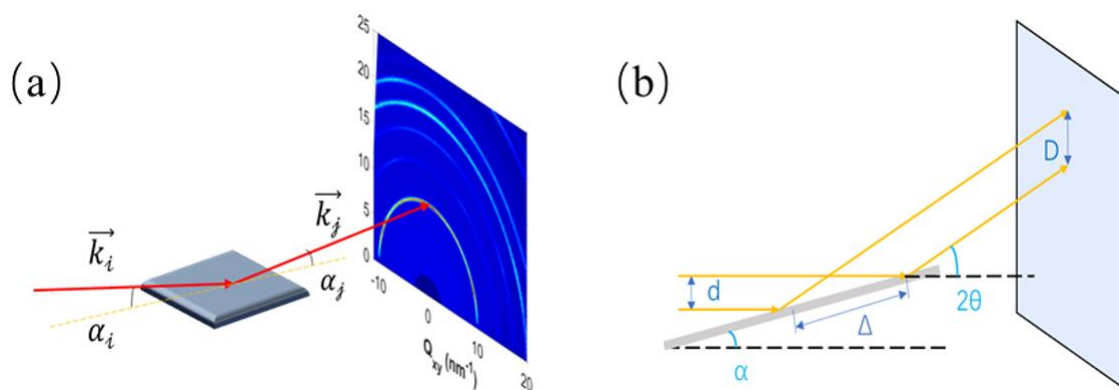


Figure 1. (a) A schematic showing the geometry for GIWAXS. (b) A schematic illustrating the footprint effects brought by the finite beam size.

Microtubular gas diffusion electrodes for electrochemical conversions

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

This work covers our recent design and fabrication of metallic Hollow fibre GDEs (HFGDEs, e.g. Cu, Sn, bronze, Ag, Bi) to tune the current density, product selectivity and performance stability. Several strategies have been applied to the catalyst layer and microstructure of HFGDE through catalyst nano-engineering (e.g. pulse or surfactant-assisted electrodeposition, electrochemical oxidation-reduction activation), in-situ alloying (e.g. formation of distinguished phase via two-step electrodeposition-annealing process), pore accessibility modification (e.g. pore size regulation and gas distribution by capillary force reduction) and reaction zone regulation (e.g. wettability regulation strategy). Similar approaches have been extended to CORR to address the carbonation and CO₂ loss issues, simultaneously enhancing reaction rate and product selectivity can be observed on the Cu nanocube-based HFGDE for yielding C₂⁺ products.

Engineering 2D Semiconductor for Valleytronics

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Van der Waals semiconductors such as 2D transition metal dichalcogenides (TMDs) are attractive for ultra-scaled and low power devices, and exploiting the novel spin-valley coupling for valleytronics [1] and quantum information processing [2, 3]. While exfoliated TMDs are expedient for quick proof-of-concept devices, the scalability for practical applications is still hindered by the lack of complete scalable processing of such materials into devices. Various traditional processes suitable for bulk semiconductors may not lend themselves directly to the fabrication of high-quality TMD devices. From electrical contacts to dielectrics for gating, the layered TMD of atomic thickness requires a near radical rethink of what are well-established rules of thumb for processing bulk semiconductors. In this talk, I'll present our efforts toward establishing scalable fabrication of valleytronic devices such as spin-valley qubits in 2D TMDs. Defects inherent and induced in the TMDs can impair their performance and hence a scientific understanding of how to handle the material defects such as vacancies, unintentional dopants, grain boundaries, and imperfect interfacing with contact or dielectric materials will be critical. I will cover our work towards understanding the role of defects, limiting the impact of oxidation of TMDs, optimizing electrical contacts and dielectric interfaces related to the fabrication of TMD devices [4 – 6]. With such efforts, we have recently achieved gate-defined quantum dot devices [6].

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Boron Nitride Nanotubes, Nanoparticles and Nanosheets: Synthesis, Properties and Applications

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Synthetic routes and electromechanical properties of pristine and carbon-doped BN nanotubes¹ nanoparticles and graphene-like nanosheets, so called “boronitrines”, are investigated. Access to properties was achieved through employing state-of-the-art methods of *in situ* and *operando* high-resolution transmission electron microscopy (TEM).¹ Elastic modulus, tensile strength,²⁻⁴ fracture toughness, conductivity of 0D, 1D and 2D BN-based nanostructures are measured in different morphologies, dimensions and defectiveness of the samples. Various modern *in situ* holders allowing for current-voltage and/or force-displacement curve measurements and shining light of various wavelengths onto the nanostructures are utilized in high-resolution electron microscope columns under atomic resolution. Based on the TEM results, emerging practical applications of BN-nanomaterials as effective supports for most common catalytic reactions, *e.g.*, CO₂ hydrogenation, CO oxidation *etc.*, hydrogen accumulation,⁵ secondary-ion batteries, reinforcing agents in light metals and polymers, and water purifiers are also shown. The results are supported by first-principle theoretical calculations.

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Collective excitations of low-dimensional materials studied with high resolution electron energy loss spectroscopy

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To understand the mechanism of how the lattice determines the physical properties of condensed matters, it is important to investigate the lattice dynamics by analyzing the phonon dispersion and lifetime. High resolution electron energy loss spectroscopy (HREELS) is a powerful tool for the measurements of phonon spectra of crystals from their surfaces.

We developed HREELS technique by introducing the hemispherical electron analyzer and realized the energy/momentum two-dimensional image detection of surface elementary excitations including phonon and plasmon [1]. By using the new HREELS, the topological nodal rings of the monolayer graphene, both dispersive and nondispersive, are identified directly [2]. The nonanalytical V-shaped phonon dispersion of the monolayer BN on Cu foils is observed, evidencing the distinct nature of the two-dimensional polar system [3]. The microscopic mechanism of the superconductivity enhancement at FeSe/SrTiO₃ interface is also clarified as the interfacial electron-phonon interaction measured by HREELS [4,5].

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Bioresponsive nanoparticles enabled catalytic therapy

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Nanomedicine has emerged as a promising approach for precision treatment of life-threatening diseases such as cancers. Nanomaterial innovation plays a key role in driving progress of the field.¹ Nanoparticle-based catalysts have been developed for catalytic nanomedicine towards safe and effective treatment of diseases.

In this talk, I will present our recent work on development of bioresponsive nanoparticles for chemodynamic, photodynamic and sonodynamic therapy by leveraging the internal or external stimuli-triggered catalytic reactions of nanoparticle-based catalysts. Our nanoparticle-based catalysts have demonstrated high catalytic activity to disproportionate hydrogen peroxide in tumors and in-situ generated hydroxyl radicals efficiently to induce apoptosis of tumor cells.² Our nanoparticles exhibited highly selective and specific anti-tumor effect. The hydroxyl radical generation-induced therapeutic effect was further enhanced by sonocatalysis and cascade catalytic reactions triggered by photocatalysis.³⁻⁵ We also showed that the nanosheet generated oxygen bubbles and promoted the long-distance and directional movement toward the tumour microenvironment, thus achieving target homing and deep penetration of the nanomedicine.⁶

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ABSTRACTS

Controlling surface chemistry to influence interfaces and induce functionality in composite materials.

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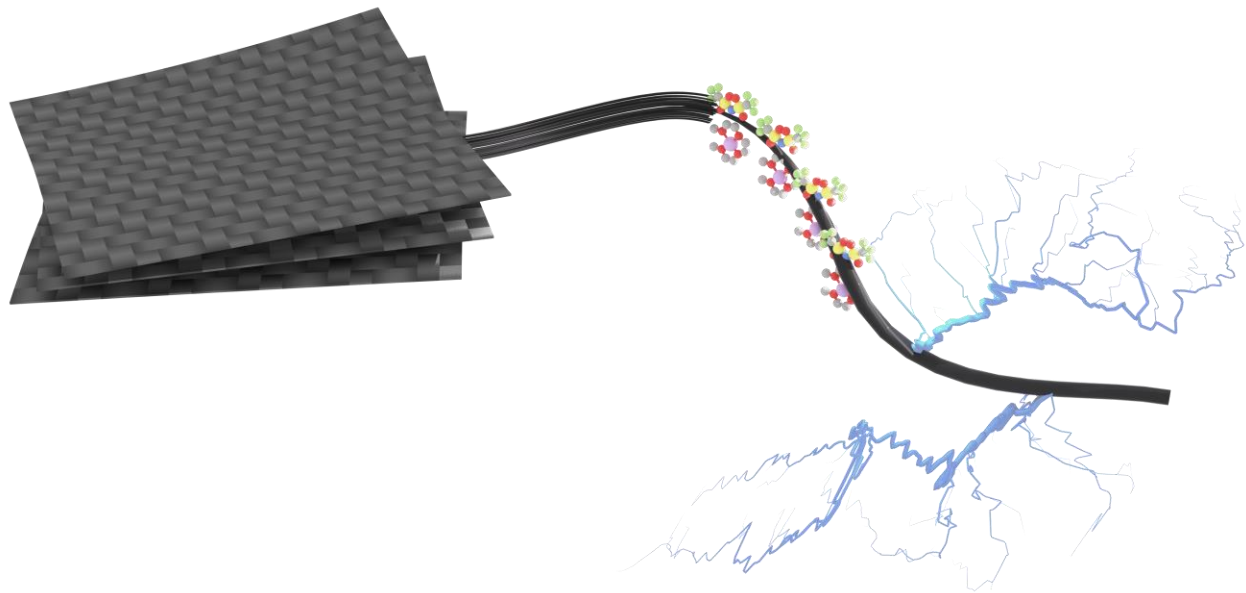
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Manipulation of a material's surface chemistry, and thereby how it interacts at interfaces, has significant ramifications on its inherent functionality (e.g. non-stick surfaces, corrosion inhibitors, etc.). In carbon fibre reinforced polymer composites, the interface between the fibre and polymer is critical to the overall performance of the part. The interfacial region is critical to the transfer of stress from the relatively weak polymer phase (typically, epoxy, nylon, polycarbonate, etc.) to the strong reinforcing fibres.

This talk will give an overview of our recent work to modify the surface of carbon fibres to install better interfacial adhesion and increase global performance measures. In addition, our efforts on the installation of functionality into a composite material will be presented. This will include a series of smaller studies that spun out of an unusual observation and serves as an excellent example of the rabbit hole that you can enter when chasing down the origin of such observations.



Quantum confinement of Dirac fermions

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In graphene quantum dots, the quantum confined Dirac fermions lead to many exotic properties. Our results indicated that we can simulate the exotic predictions of quantum electrodynamics in graphene quantum dots [1-3]. For example, we demonstrated that whispering-gallery modes and atomic collapse states can coexist and change mutually in a graphene quantum dot. Moreover, our experiments demonstrated that we can realize exotic electronic properties beyond the parent material, i.e., the graphene, in graphene quantum dots [4-10]. In this talk, I will introduce two examples. One is the tunable Berry phase and quasibond states in graphene quantum dots [4,5]. The other is novel effects of local rotational symmetry-breaking potentials on the quantum confined states. Our study indicated that the scatterings between different orbital angular momentum states in rotational symmetry-breaking potential can generate additional phase singularity [10]. Moreover, the anisotropy of confining potential induces the *sd* hybridization between two quasibound states, which are also an atomic collapse state and a whispering gallery mode, in graphene quantum dots [11].

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Hydrogen-rich bond (N-H and B-H) for Energy Storage and Transfer

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Hydrogen-rich systems consisting of light elements such as B, C, and N have been extensively studied as hydrogen storage materials. In this talk, I will first give a brief overview of borohydrides for hydrogen storage, which includes NaBH_4 and MgBH_4 . I will then discuss reactions between amine-borane complexes and amines which generate high purity H_2 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 NaBH_4 and H_2O at room temperature. 1,6;2,3-bis-BN cyclohexane, an isostere of cyclohexane with two adjacent BN pairs, was recently synthesized in our laboratory. Its ring flipping barrier is similar to that of 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. Lastly, I will introduce our latest research on electrolysis of ammonia/water solution to produce green hydrogen and nitrite/nitrate.

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Towards Perovskite Solar Windows

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Transparent photovoltaics are garnering significant interest for power generation in applications requiring building integrated photovoltaics (BIPV), including solar windows and other shading elements. Metal halide perovskites have emerged as one of the most lucrative material classes for such device architectures due to their exceptional optoelectronic properties, compositional versatility enabling a wide range of transparency levels, and low power to weight ratio. This talk will delve into two main perovskite device architectures that have prospects to revolutionise BIPV: semi-transparent and semi-opaque perovskite solar cells.

Semi-transparent perovskite solar cells (ST-PeSCs) are promising solar window candidates owing to their potential high efficiency and visible transmittance compared to traditional amorphous silicon analogues. However, their technological infancy still presents challenges in terms of poor long-term device stability and non-optimal efficiency. Interfacial engineering and bulk compositional variation within the A and X sites of the ABX₃ hybrid organic-inorganic perovskite structure are considered as two key pathways to achieve both increased device performance and stability [1,2]. Through this approach, record power conversion efficiencies with high stability factors are achieved for ST-PeSCs.

Conventionally, ST-PSCs are realised by thinning the perovskite absorber layer to allow partial light transmission, while also replacing the opaque back electrode with one that is transparent. This approach yields devices with a perceived colour (typically red to yellow) due the perovskite optical bandgap being within the visible range. A pathway to overcome this hurdle is by patterning the solar cell in a way that selected regions are entirely transmissive, while others remain fully absorbing [3]. Such semi-opaque perovskite solar cells (SO-PeSCs) can support greater efficiencies and colour purity levels than ST-PSCs. Here, we explore the development of such novel device architectures using hydrophobic templating [4]. Compared to literature benchmarks, these devices are on-par with the best performing ST-PeSCs reported to date, while exhibiting the highest efficiency for color-neutral perovskite solar cells over a wide transparency range.

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Heterogeneous Molecular Catalysis for Electrochemical CO₂ Reduction

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Electrochemical reduction of CO₂ in aqueous electrolytes is one of the most promising routes for commercial CO₂ utilization. A switch from the currently used noble metal-based catalysts to the carbon-supported macrocyclic complexes could bring a much-needed cost reduction thus making the technology economically viable. However, the inherently low conductivity and tendency of molecular catalysts to degrade during the long-term operation present a challenge for catalyst design. We applied mechanistic investigations to tackle a challenging problem of the catalyst durability in CO₂ electrolysis. It was determined that the loss of activity takes place due to the reductive carboxylation and co-occurring formation of inactive metal complex. Therefore, the stability could be greatly enhanced through the introduction of bulky donating substituents around the macrocyclic core. These insights allowed us to design and synthesis a catalyst bearing eight methoxy groups around the lateral aromatic moieties which demonstrate no noticeable degradation during the repetitive long run electrolyses. These design principles, combined with our recent development of bicarbonate electrolysis and heterogeneous molecular catalysts, would provide a low-cost and very stable catalytic system for CO₂ electrolysis.

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Material design to make organic radical batteries more practical

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The rapid advent of portable and flexible devices has spurred major advancements in flexible energy storage for seamless integration. It thus requires new, lightweight, easily processed, mouldable, and flexible materials. Unfortunately, traditional metal and inorganic materials could not fulfill all the requirements. In addition, the ever-increased consumption of metal-based batteries has led to a sustainability concern, such as the depletion of rare metal resources and potential environmental and health impacts - if not properly recycled. Batteries made from organic redox polymers represent a promising and viable solution to the next generation of sustainable energy storage systems. Nitroxide radical polymers (NRPs) are some of the most promising redox polymers, providing corresponding batteries with high voltage, fast charging, and long cyclability.[1-3] Despite the attractive properties of NRPs as active electrode materials, these polymers have limited implementation in battery-powered electronic devices or large-scale energy storage. One of the greatest challenges is their low energy storage capability (i.e., 110 mAh/g). For example, most studies on radical polymer batteries could only realize the oxidation process (i.e., TEMPO^{+/•}) for battery applications due to the sluggish kinetics of the reduction process (i.e., TEMPO^{•/0}), which greatly compromises their energy storage capability. Recent research reveals that two-electron storage might be achieved if polymer structures, polymer/nanocarbon composites, or electrolytes are carefully designed.[4] In recent years, our group has explored how the chemical structures of polymers and physical morphologies of electrode composites dictate the electrochemical properties of the NRP cathode, implying that a rational design of radical polymer electrodes could enhance energy storage performance (Fig. 1).[5, 6] Our group has successfully applied NRPs as cathodes for a range of hybrid batteries, including those using Li, Na, K, Al, and Zn, demonstrating the versatility and practicality of these materials in various energy storage applications.[7-9]

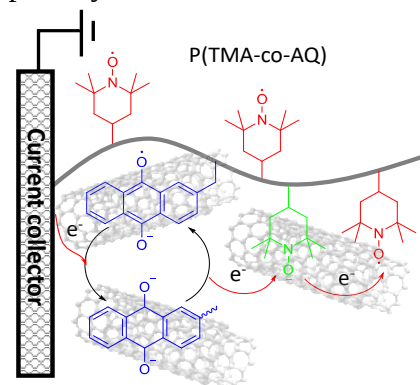


Figure 1. AQ-catalysed two-electron storage of nitroxide radical polymers

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Molecular Modelling of Electrocatalyst Materials for Clean Energy Conversion

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

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

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Advanced Materials Capabilities at the Australian Synchrotron

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The Australian Synchrotron is a government-funded user facility that plays a pivotal role in advancing research across multiple scientific disciplines, with *advanced materials* research, particularly in catalysis and energy storage, now accounting for about 50% of research conducted. This presentation will highlight key beamline techniques relevant to these areas, including diffraction, imaging, and spectroscopy. State-of-the-art beamlines provide essential insights into the structure, properties, and performance of materials across various scales, from atomic to macroscopic levels. For instance, the X-ray Absorption Spectroscopy (XAS) beamline enables researchers to leverage in-situ and operando techniques to investigate real-time processes critical to catalysis and energy storage [1, 2]. Case studies will demonstrate how synchrotron-based research drives outcomes, positioning the facility as a crucial resource for developing next-generation materials.

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ABSTRACTS

Ferroelectric Dynamics in 2D function materials: Insights from Machine learning enabled large-scale simulations

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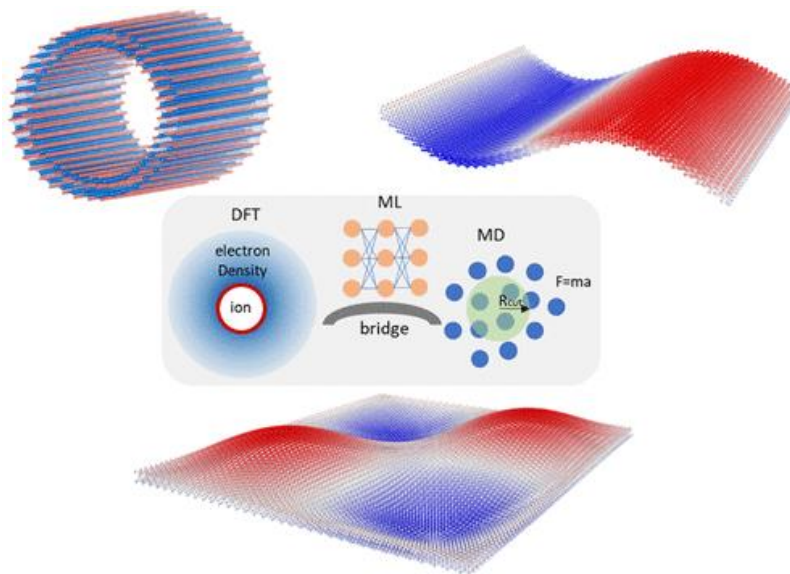
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Understanding ferroelectric dynamics, such as polarization switching and domain formation under complex strain, temperature, and electric field conditions, is crucial for the design of advanced ferroelectric devices. However, atomic-level investigations in this area have been limited due to the constraints of traditional theoretical methods. In this presentation, I will discuss the development of a deep-learning potential based on neural network machine learning, which facilitates large-scale simulations of ferroelectric dynamics.

Two significant studies will be highlighted. First, we explore the effects of bending, rippling, and bubbling on ferroelectric domains in an In_2Se_3 monolayer. Due to the strain-dependent switching energy barriers, we observe automatic polarization reversal in $\alpha\text{-In}_2\text{Se}_3$ under these deformations, leading to the creation of localized ferroelectric domains of varying sizes. The switching dynamics are influenced by both the magnitude of curvature and the ambient temperature.

In the second study, we investigate the switching barrier associated with antiferroelectric-ferroelectric interlayer coupling in bilayer ferroelectric CuInP_2S_6 , revealing a dependence on stacking configurations. By twisting the bilayer, we can effectively create ferroelectric domains. The stability, size, and switching dynamics of these domains are significantly affected by the twisting angle, environmental temperature, applied strain, and external electric field.



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Pure-water-fed electrocatalytic CO₂ reduction to valuable chemicals

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Renewable electricity-powered electrochemical CO₂ reduction (ECO₂R) shows promise for producing valuable fuels and feedstocks, but the selective generation of economically desirable products like ethylene (C₂H₄) is challenging. C₂H₄ is crucial for plastics, solvents, and cosmetics, and there is currently no direct CO₂ reduction to C₂H₄ in the chemical industry. The main obstacle to ECO₂R is carbonate formation, leading to low carbon conversion, high energy usage, and poor system stability in alkaline and neutral reactors. A new pure-H₂O-fed membrane-electrode-assembly (MEA) electrolysis system for ECO₂R-to-C₂H₄ using a high-performance step-facet-rich Cu catalyst is presented. This system eliminates carbonate formation and crossover. ECO₂R was scaled up in a 6-MEA-cell stack with a total current of 10 A under pure H₂O, achieving a Faradaic efficiency of ~50% toward C₂H₄ and a system lifetime of over 1000 hours [1].

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Chemical Cascades Catalysed by Earth Abundant Elements

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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 [2]. Multifunctional heterogeneous catalysts are an effective strategy to drive chemical cascades [3,4], with attendant time, resource and cost efficiencies by eliminating unit operations arising in normal multistep processes. Despite advances in the design of such catalysts, the fabrication of proximate, chemically antagonistic active sites remains a challenge for inorganic materials science.

Hydrogen-bonded organocatalysts offer new opportunities for the molecular level design of multifunctional structures capable of stabilising antagonistic active sites. We report the catalytic application of a charge-assisted, hydrogen-bonded crystalline material, bis(melaminium)adipate (BMA), synthesised from melamine and adipic acid, which possesses proximate acid-base sites [5]. BMA exhibits high activity for the cascade deacetalisation-Knoevenagel condensation of dimethyl acetals to form benzylidenemalononitriles under mild conditions in water (**Figure 1**); BMA is amenable to large-scale manufacture and recycling with minimal deactivation. Computational modelling of the melaminium cation in protonated BMA explains the observed catalytic reactivity, and identifies the first demethoxylation step as rate-limiting, in good agreement with time-dependent ¹H NMR and kinetic experiments. A broad substrate scope for the cascade transformation of aromatic dimethyl acetals is demonstrated.

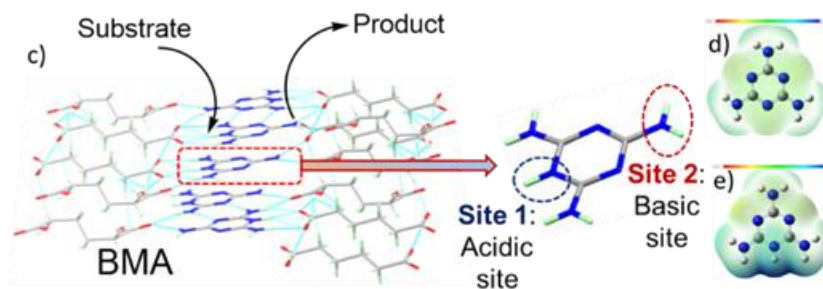


Figure 1. Cascade deacetalisation-Knoevenagel condensation of dimethyl acetals over BMA.

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Advanced 2D nanomaterials for water and energy conversion

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Water source pollution and energy shortages are serious global challenges. Researchers worldwide are seeking to improve water purification or clear water generation and renewable energy harvesting strategies to guarantee environmentally sustainable development. To address the dual challenges of generating renewable energy and sustainable water, we have developed novel functional nanomaterials that can harvest energy from the ocean and separate molecules and ions, remove organic pollutants, and generate freshwater from seawater and industry wastewater for potential applications in both future energy and water generation.

Here, we have reported a series of functionalized 2D nanomaterials and their membranes such as graphene, BN, MoS₂, MXene, metal nitrides with unprecedented performance in multipurpose molecular and ion sieving in water and in organic solutions with high permeation and selectivity, high rate of ionic transport for energy generation, and broadband (UV-visible-Infrared) light absorption and excellent photothermal conversion efficiency for freshwater generation. Such multipurpose and super stable advanced nanomaterials with high throughput manufacturing route facilitates the innovative application of 2D nanomaterials to meet the rapid industrial development multi-demands.¹⁻⁸

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Nanobiohybrid materials for environmental sustainability

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

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

In-Situ Transmission Electron Microscopy Investigation of Ferroelectric Domain Switching Behaviour

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Ferroelectrics results from the displacement of ions that leads to spontaneous polarisation with the internal electric field pointing towards a specific direction in materials. A region with the same polarization direction is called a ferroelectric domain. Understanding ferroelectric domain switching behaviour under external stimuli is crucial for the applications of ferroelectrics in memories, actuators and nanoelectronic devices. In this presentation, I will present our recent in-situ transmission electron microscopy investigation results on how separate and combined mechanical and electrical loadings affect ferroelectric domain structures and how ferroelectric fatigue occurs. Our results show that mechanical confinement during electrical loading adds one more degree of freedom for domain manipulation [1], which would provide an appealing possibility for significantly improving ferroelectric device performance, and that charge accumulation at domain walls is a major mechanism leading to ferroelectric degradation [2].

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Coordination Engineering in Nanomaterials Design for Energy Applications

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Nanomaterials have attracted an increasing attention for their unique properties which cannot be obtained from the corresponding bulk forms, such as super-high chemically reactive surfaces, rapid “in-plane” charge transport, significant quantum-confinement effect, etc. In this presentation, nanomaterials and their hybrids design using coordination engineering strategies has been studied, with the aim of understanding the nature and mechanisms of their electronic coupling, charge transfer, and catalytic activity in hydrogen evolution reactions (HER), oxygen evolution reactions (OER), and dissociative adsorption reaction of small molecules. Low dimensional nanomaterials and their hybrids, which promote electronic coupling and efficient charge separation arise from the effects of adsorbent nature, quantum size engineering, and defect assistance, are therefore boost their promising energy correlated applications.

Probing the Charge Carrier Dynamics and Trap Features of Solution-Processed Semiconductors via Time-Resolved Spectroscopy

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Along with the remarkable progress in the field of organic, quantum dots-based and perovskite optoelectronics, solution-processed semiconductors have shown unprecedented successes. However, the characterization of these novel semiconductors is very challenging due to the highly disordered structure, dispersive charge transport, low conductivity and relatively short carrier lifetimes. In this talk, I will present the optoelectronic characterization of these novel materials systems, mainly via time-resolved spectroscopy, *e.g.*, microwave conductivity (TRMC), transient absorption (TA) and deep-level transient spectroscopy (DLTS). I will start with the basic principle and the set-up of these techniques. Then, I will focus on the optoelectronic properties obtained from the transient decays, including real and imaginary conductivity at GHz region, mobility, recombination rates, shallow or deep-level trap density and charge carrier lifetimes. At the end, I discuss the key challenges facing these techniques. I will also point out the opportunities, which are promising to explore and may require more research activities.

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Electrochemistry of Carbon Materials

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As a bridge between secondary batteries and electrochemical capacitors, hybrid charge storage devices are considered promising for simultaneously achieving high energy, power, and long cycling. However, limited by the difference in charge storage mechanisms and the strong coupling relationship between various properties, it is difficult to exert the advantages of cathode and anode in all cases. To this end, we proposed a transformative discussion on how to maximize the performance of hybrid charge storage devices from an electrochemical perspective. During the discussion, the zero-voltage potential was found to be the key to balance the capacity of the cathode and anode, and the self-matching of potential that we proposed and defined was the key that affects the dynamic electrochemical process. Combining electrochemical behaviour, testing methods, and electrode materials, we performed an exhaustive analysis of the coupling and matching of ideal hybrid charge storage in terms of capacity, kinetics and cycle life. In addition, considering the diversity of practical electrochemical systems, we also discussed the more complex electrochemical behaviours involved and the corresponding specific coupling and matching relationships. The differences in electrodes mean that coupling and matching are unavoidable for any charge storage system. More importantly, the corresponding theoretical research means that the electrochemical behaviour can be modelled and analysed by machine learning to predict the overall performance of the device and optimize the design based on the collected data. Our analysis, discussion and insights provide new an idea and direction for the research and development of hybrid charge storage and other systems.

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Empowering Electrochemical Biosensors by Nanocomposite Materials for Biomarker Detection

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The 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 MXene-based nanocomposites for electrochemical sensors that enable unprecedented performance in terms of biomarker detection. 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.

Sustainable Quantum Materials

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Quantum technologies underpinned by functionalized quantum materials are poised to transform our life. In this technology development, it is important to use ‘Benign by Design’ and Green Chemistry principles early to ensure sustainability is built in right from the start. In this talk, I will introduce carbon quantum dots, particularly waste-derived carbon dots, as one of the promising sustainable quantum materials for various advanced technologies.^[1-4] I will use photocatalysis for energy and chemical production, and chemical sensing at excited state as examples to illustrate the circularity and application potential of carbon quantum dots.

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ABSTRACTS

The Progress of “Materials Turing Scheme”: Developing AI Public Platforms for the Automatic Design of Energy Materials

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This talk will present the current progress of the “Materials Turing Scheme” led by the Hao Li Lab at Tohoku University, in collaboration with >100 researchers from >20 universities including The University of Sydney, The University of Queensland, and The University of Adelaide. The current stage of the “Materials Turing Scheme” includes the successful development of a wide range of energy materials databases, including the Digital Catalysis Platform (*DigCat* [1], the first-ever digital catalysis platform and electrocatalysis database, including >0.4 million experimental and >0.3 million computational data), the hydrogen storage materials database developed in collaboration across the research teams in Japan, thermoelectric materials database, and the dynamic databases of solid-state electrolytes and polymer electrolytes (DDSE & DDPSE [2]). Based upon these databases, we offer dynamic data visualization, precise literature tracking, an intelligent Q&A assistant, cutting-edge tools for predictive microkinetic modeling, AI chatbot based on materials data and knowledge, on-the-fly machine learning force field training, and regression model development. This talk will particularly focus on discussing how to use these AI public platforms to realize an automatic design of catalyst and hydrogen storage materials.

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Waste Reforming for Cogeneration of Green Hydrogen and Chemicals

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Climate change caused by carbon emission is a global challenge that necessitate urgent action and lead to the sustainability shift towards low-carbon biofuels, renewable energy, and clean hydrogen fuel, as well as green chemicals. High purity hydrogen can be generated from water electrolysis but is hindered by kinetically sluggish oxygen evolution reaction (OER) and the safety issue caused by possible explosive mixture of oxygen and hydrogen under the condition of partial loading and membrane degradation. There is a widespread effort to replace OER with the more favorable electrooxidation of small organic molecules. Although value-added products can be generated, the production of these organics is process-intensive and costly. Most importantly, they lack the abundance necessary to meet the requirements of a hydrogen economy.

Abundant raw biomass with annual production of billions of tons in nature are promising alternatives to these small organics. Significantly, biomass reforming via electrooxidation (to replace OER) could close the carbon cycle and promote a circular economy. However, the complex structure of raw biomass poses challenges, limiting processability. Consequently, these biomass materials are conventionally used as fuel for electricity generation, leading to CO₂ emission and underutilization of biomass. Therefore, from both resources recovery and carbon abatement perspectives, it is critical to develop advanced electro-refinery system for biomass valorisation. To overcome the low processability of raw biomass, highly efficient pretreatment methods were developed and thoroughly investigated.

Biomass wastes were featured as promising reactants for reforming due to their abundance and availability. Without proper handling, these waste release carbon back into the atmosphere only after a short period of storage, rendering advanced carbon storage and utilization crucial. Reforming of biomass waste not only produces green commodity chemicals and hydrogen fuels but also holds promising potential for climate change mitigation. Herein, I will summarize our recent works [1-9] on reforming various wastes to green hydrogen and chemicals.

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ABSTRACTS

Design and In-Situ Analysis of Metal-Based Electrocatalysts for Clean Energy Conversion

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In this presentation, we examine the pivotal role of heterogeneous electrochemical processes occurring at electrode interfaces in the realms of clean energy conversion, storage, and utilization. A key challenge in this field lies in the development of high-performance inorganic electrocatalysts capable of maintaining electrochemical activity under operando conditions. Addressing this challenge requires a comprehensive understanding of the structural, crystalline, and electronic properties of these electrocatalysts during active operation. We will discuss the deployment of advanced in-situ characterization techniques, including X-ray Absorption Spectroscopy (XAS), X-ray Diffraction (XRD), and Raman spectroscopy, to elucidate the active states and performance of metal-based catalysts (involving transition metals such as Mn, Fe, Co, Ni, Cu, Ru, Bi, and Ag) for critical electrochemical reactions. These reactions include the Oxygen Reduction Reaction (ORR), Oxygen Evolution Reaction (OER), Hydrogen Evolution Reaction (HER), and Carbon Dioxide Reduction Reaction (CO₂RR). In particular, we will delve into the electrochemical transformations of these catalysts from their precursor states to their activated forms. The observed enhancements in electrocatalytic activity are attributed to the electronic modulation of transition metals by their substrates and the distinctive chemical environments present within the nanoscale structures.

Sustainable Photocatalytic Production of H₂O₂ over Phenolic Resins Catalysts

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Hydrogen peroxide (H₂O₂), one of the most important 100 chemicals, is widely involved on most occasions in daily life. The photosynthesis of H₂O₂ via oxygen reduction reaction (ORR) and water oxidation reaction (WOR) has been advocated in recent years, which alleviate the environment and energy crisis as well as satisfy on-demand production and in situ applications. Designing polymeric photocatalysts at the molecular level to modulate the photogenerated charge behavior and catalytic reaction kinetics is a promising and challenging strategy for efficient H₂O₂ photosynthesis. Recent researches on the phenolic resin-assisted photocatalytic generation of H₂O₂ relies on resorcinol-formaldehyde (RF523) catalysts with alternating donor-acceptor structures. We optimized RF523 resins from the perspective of molecular design for promoting charge separation, such as regulation of donor/acceptor ratio,[1] improvement of spatial charge distribution,[2] modification of quantum dots or graphene.[3, 4] In addition, we developed a benzoxazine-based phenolic resin as exceptional photocatalyst beyond RF523 for long-term (>72 h) photocatalytic H₂O₂ production.[5] Aldol condensation, Mannich reaction and cyclization condensation impel the formation of m-aminophenol-formaldehyde resin (APFac) at ambient conditions, avoiding the costly precursors as well as tedious and hazardous preparation process of photocatalysts. Benzoxazine structure was identified as the crucial photocatalytic active segment in APFac. Favorable adsorption of oxygen/intermediates on benzoxazine structure and commendable product selectivity accelerated the reaction kinetically, thus endowing APFac catalysts superior H₂O₂ yield than most polymeric photocatalysts under visible-light without sacrificial agents.

Our works explore the potential and prospect of phenolic resins in H₂O₂ photosynthesis and shed light on the de novo design and analysis of metal-free polymeric photocatalysts.

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Porous Carbon Based Composites for Energy Storage and Conversion

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Abstract

It is universally recognized that a dependence on foreign oil and/or gas creates national vulnerabilities and endangers social stability. Moreover, the gaseous emissions from the burning of fossil fuels and biomass are not only polluting the air of cities but are also creating a global warming with alarming consequences. In response to the impending energy crisis, many countries are once again focusing on national efforts to reassess the use of alternative energy sources and replace the internal combustion engine with wireless electric motors. Thus, it is essential to develop new materials or technologies to enhance the electrochemical performance of energy storage and conversion systems. Porous carbon-based materials have garnered significant attention due to their unique structures and electrochemical properties, making them suitable for energy storage and conversion devices. In this context, we summarize several materials used in various applications, such as lithium-ion batteries, lithium-sulfur batteries, and lithium-oxygen batteries. The findings indicate that these porous carbon-based materials exhibit outstanding electrochemical performance thanks to their enhanced conductivity and reactivity. This contribution provides valuable insights for improving low-conductivity nanostructured materials in energy storage and conversion applications.

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Tunable Ferroelectric Topological Defects on 2D Topological Surfaces: Complex Strain Engineering Skyrmion-Like Polar Structures in 2D Materials

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Polar topological structures in ferroelectric materials have garnered significant interest due to their intriguing physical properties and potential applications in high-density, non-volatile memory devices. While most polar topological patterns are typically observed in bulky perovskite superlattices, this presentation introduces the discovery of tunable ferroelectric polar topological structures in two-dimensional (2D) PbX (X = S, Se, Te) materials. This breakthrough is achieved through topological strain engineering, integrating first-principles calculations, machine learning molecular dynamics (MD) simulations, and continuum modelling. Our first-principles calculations reveal that strain-induced, reversible ferroelectric phase transitions in these 2D materials exhibit diverse polarization directions strongly correlated with the applied strain. Leveraging the mechanical flexibility of 2D PbX, MD simulations demonstrate that complex strain fields, generated by mechanical indentation, can produce unique skyrmion-like polar topological vortex patterns. Continuum simulations, scaled to experimentally accessible dimensions, further uncover various skyrmion-like structures—including vortices, anti-vortices, and flux-closure patterns—that can be dynamically transitioned between by designing different types of mechanical loadings, such as out-of-plane indentation or air blowing. The ability to engineer and control reversible polar topological structures in flexible 2D materials opens up exciting opportunities for the next generation of nanoelectronics and sensor devices, marking a significant advancement in both fundamental research and technological applications.

Advanced nanomaterials for thermal energy harvesting and energy storage

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To tackle the energy shortage and meet the growing demand for portable and wearable electronic devices like flexible sensors and smart clothing, there's been a notable rise in interest towards designing flexible renewable energy devices with excellent heat dissipation. This emerging trend not only aims to fulfill the demand for sustainable power sources but also aligns with the evolving landscape of consumer electronics. Novel two-dimensional (2D) nanomaterials have unique properties, including exceptionally high specific surface area, customizable physical attributes, rich surface chemistry, superior mechanical strength, and ease of processing. These advancements present a promising avenue for the design and development of flexible renewable energy devices. Here, we report functional 2D nanomaterials-based composites materials with multifunctional properties, which exhibit highly potential applications in high-performance flexible electrically insulating substrates and flexible energy storage.¹⁻⁵

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Electrolyte Engineering for Wide-Temperature Lithium Metal Batteries

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With the fast development of electronic devices, the requirements on batteries with high-energy and all-temperature are urgently needed. Rechargeable lithium-metal batteries (LMBs), are considered as compelling substitutes for conventional lithium-ion batteries in near future due to their high energy-density contributed by the high theoretical capacity (3,860 mAh g⁻¹) of Li metal anode (LMA). However, Li anode with a low standard electrode potential of -3.04 V (versus the standard hydrogen electrode) is so energetic that it can easily react with traditional carbonate electrolytes, resulting in uncontrolled side reactions and dendrite growth. To address these issues, a stable and efficient electrode/electrolyte interphase (EEI) is keen to established in LMBs. The solvated Li⁺ structure has significant influence in EEI components. How to rationally design electrolyte chemistry to affect the solvation structure, and finally influence the EEI is quite important. In our work, a series of strategies have been developed to achieve this delicate design on solvation chemistry, and thus obtain advanced EEI, and simultaneously reduced desolvation energy on interphase. The enhanced Li⁺ diffusion kinetics through tuning solvation structure not only prolongs the life-span of LMB, but also empowers LMB working functionally in a wide temperature range (-20~60 °C); which will boost the practical application of high-performance LMB in real world.

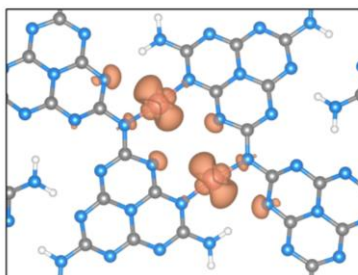
Geminal-atom catalysis: next frontier in sustainable chemical manufacturing?

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A global shortage of energy and resources, and the push for clean manufacturing processes, means that economical and sustainable production methods of fine chemicals and pharmaceutical are urgently needed. Transition-metal-based catalysts are critical for developing molecular complexity in organic syntheses, typically exploit homogeneous organometallic complexes. Despite their unparalleled synthetic capability, concerns arising from using homogeneous catalysts include their potentially high production costs, the environmental impact associated with challenges in product separation and purification, and catalyst recycling. The development of heterogeneously catalysed processes is highly attractive for large-scale production to facilitate catalyst separation, recovery and reuse, and improve adaptability for continuous-flow synthesis. Single-atom catalysts (SACs) have well-defined active sites, making them of potential interest for organic synthesis. However, the architecture of these mononuclear metal species stabilized on solid supports may not be optimal for catalysing complex molecular transformations owing to restricted spatial environment and electronic quantum states. In this talk, I will introduce a new class of heterogeneous geminal-atom catalysts (GACs), which pair single-atom sites in specific coordination and spatial proximity. These advancements go beyond single metal centers, paving the way for the development of next-generation atomic-precision catalysis with potential to transform the landscape of chemical production and energy conversion for a more sustainable future.



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Giant electrocaloric strength generated by the polarization flip in PMN-PT single crystals and boosted energy storage densities in lead-free $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ -based thick film ceramics

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Electrocaloric effects (ECEs) of [110] and [111] oriented PMN-PT single crystals were studied in the temperature range of 293–423 K. The Maxwell relations and Landau-Ginsburg-Devonshire (LGD) phenomenological theory were employed as the indirect method to calculate the electrocaloric properties, while a high resolution calorimeter was used to measure the adiabatic temperature change of electrocaloric effect directly. The results indicate that the directly measured temperature changes of $\Delta T > 2.5$ K at room temperature were procured when the applied electric field was reversed from 0 to -1 MV/m, which are > 4 times larger than that with electric changes from 1 MV/m to 0, and also larger than those calculated pursuant to the Maxwell relation, and the LGD theory in the temperature range of 293 – ~ 380 K. In addition, a new type of lead-free $(0.74-x)\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$ - 0.06BaTiO_3 - 0.2SrTiO_3 - $x\text{Bi}(\text{Mg}_{0.5}\text{Zr}_{0.5})\text{O}_3$ (NBT- x BMZ) relaxor ferroelectric thick film ceramics were designed and prepared via compositional and microstructural optimization. Doped $\text{Bi}(\text{Mg}_{0.5}\text{Zr}_{0.5})\text{O}_3$ (BMZ) effectively widened the bandgap, introduced polar nanoregions, enhanced the relaxor ferroelectric characteristics, improved the impedances, and ultimately improved the dielectric breakdown strength (DBS) as well as the ESP. As confirmed by both the selected area electron diffraction patterns and the Rietveld refinement of X-ray diffraction patterns, multiphase coexistence structure was successfully constructed, resulting in merged polarization and delayed polarization saturation. Multiphase coexistence structure, pinched polarization-electric field hysteresis loops and ultrahigh DBS collectively boost the ESP. Remarkably, a recoverable energy storage density of 15.79 J/cm^3 and an energy storage efficiency of 92.86% were achieved in NBT-0.22BMZ thick film. Benefiting from the microstructural tailoring, excellent thermal stability (20–160 °C), frequency stability (1–200 Hz), and fatigue endurance ($> 10^4$ cycles) were realized for the same composition. Additionally, the NBT-0.22BMZ thick film also exhibited a large power density of 582.47 MW/cm^3 and an ultrafast discharge speed of ~ 44.0 ns. This work provides a novel strategy to develop next-generation dielectric capacitors with superior energy storage properties for applications in advanced pulse power systems.

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Two-dimensional Unconventional Ferroelectricity

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Ferroelectric materials, particularly ferroelectricity in two-dimensional systems, have attracted significant interest over the past few years. However, nearly all reported ferroelectric materials are compounds composed of different types of atoms. Recently, despite being counterintuitive, we reveal spontaneous polarization and ferroelectricity in two-dimensional elemental group-V materials with a buckled lattice structure similar to black phosphorus, based on first-principles calculations and confirmed by experimental measurement. Additionally, we develop a general model to understand and search for potential two-dimensional ferroelectric and antiferroelectric materials. Using this model, we also discover that ferroelectric and antiferroelectric phases can exist in group-IV and group-VI elemental two-dimensional systems. More importantly, two-dimensional element ferroelectric materials exhibit anomalous negative piezoelectric coefficients and intrinsically stable charged domain walls, making them promising candidates for ultrathin ferroelectric devices with broad application prospects. The conclusions drawn from the study of elemental ferroelectric systems suggest the possibility of realizing unconventional ferroelectric effects in other ferroelectric systems, holding great potential for experimental realization and practical applications.

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Functional materials for Multivalent Metal Batteries

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

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Selective Extraction of Critical Metal Resources from Spent Li-ion Batteries

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The age of the electric car is all but upon us. Lithium-ion batteries (LIBs) are among the costliest components of electric vehicles (EVs). Along with the boom of global EV market, billions of LIBs are reaching their expected lifetime. Additional to problems of environmental care and safety, the metals and materials used in LIBs will be lost if not properly handled. Environmental pollution and critical materials loss from spent LIBs is thus a major global concern. Recycling of spent LIBs is urgently needed to address the raised significantly economic and environmental concerns, but traditional recycling pyrometallurgy and hydrometallurgy technologies are not efficient and sustainable. Another challenge in the practical LIB recycling is the selective separation and recovery of multiple metallic elements in the cathode materials. In this talk, I will introduce our recent work on the design of a leaching and separation process system based on the “green solvents” to enable the high selective recovery of transition metals and Li from spent LIB cathode [1-3]. Compared to the traditional hydrometallurgy technologies using strong acid and pyrometallurgy using high temperature, the process is low cost and recyclable, and avoids using extreme heat or corrosive acids.

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Layered hexagonal metal oxides – A new member of 2D family

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In the past decades, two-dimensional materials have attracted extensive research interest. Materials of graphene and its analogues (including group V elements, metalenes), transition metal - dichalcogenides (TMDs), group III monochalcogenides, transition metal carbides as well as nitrides have been widely explored. These atomically thin materials have exhibited unique light-matter interactions, quantum effect and other physical properties. Among the 2D family, the bulk non layered metal oxides are hardly exfoliated into 2D. Despite the promising properties of 2D metal oxides, the practical realization of these benefits relies heavily on the successful synthesis of high-quality, well-controlled 2D layered structures. Recent advancements in synthesis techniques have significantly contributed to this effort. The methods used to produce 2D metal oxides can be broadly classified into three key approaches: top-down exfoliation, bottom-up synthesis, and the liquid metal strategies. Recently, our team has developed an artificial growth of metal oxide thin films from the metal-oxygen interface, that the metal oxides are naturally created in a layered hexagonal phase and allow mechanical exfoliation into 2D with ease. The finding has been demonstrated to be applicable across a variety of metal categories including transition metals, post-transition metal, semi-metal and lanthanides. In the presentation, I will discuss recent research advancements and provide an overview of our previous work in the field of metal oxide-based sensing technologies.

Controllable Electronic Quantum Phases in 2D Metal-Organic Materials

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Strong Coulomb interactions between electrons in materials can lead to a vast range of exotic quantum phenomena, including metal-to-insulator transitions, diverse magnetically ordered phases, and even superconductivity. These properties depend strongly on the chemical potential of the material, that is, on the occupancy of the material's quantum mechanical electronic states.

This means that tuning of the material's chemical potential – for example, by applying a gate voltage, as in a semiconductor-based field-effect transistor – allows for control over and reversible switching between such diverse quantum phases. As such, materials hosting strong electron-electron interactions can act as functional materials in voltage-controlled devices, offering enticing prospects for applications in electronics, spintronics, and information processing and storage.

In particular, two-dimensional (2D) materials with specific crystal structures – such as the kagome crystal structure, where atoms or molecules are arranged in corner-sharing equilateral triangles – can be characterized by an electronic band structure that includes flat electronic bands, which can enhance electronic interactions. For a specific electron occupancy of such a band structure, the material can behave as an insulator, with a significant insulating bandgap. For other electron occupancies, the material can behave as a metal.

Here, I will present results on an atomically thin 2D metal-organic framework consisting of flat aromatic molecules (9,10-dicyanoanthracene; DCA) arranged in a kagome structure via coordination with metal atoms (copper; Cu). Metal-organic frameworks (MOFs) are hybrid materials whose properties can be tuned through careful selection of the constituent organic molecules and metal atoms. As such, there has been growing interest in MOFs as functional electronic nanomaterials.

When synthesized on a weakly interacting metal [1], this specific 2D kagome MOF hosts local magnetic moments, as revealed by low-temperature scanning tunneling spectroscopy. Density functional theory and mean-field Hubbard modelling show that these magnetic moments are the consequence of strong electron-electron Coulomb interactions given by the kagome arrangement of the organic molecules within the 2D MOF. On an insulator – such as hexagonal boron nitride (hBN) – the same 2D kagome MOF exhibits a ~200 meV electronic bandgap which is consistent with dynamical mean-field theory predictions of an insulating phase given by strong electronic interactions [2]. Relying both on the local work function variations of the substrate and on the electric field applied by the tip of a scanning probe microscope, the occupancy of the electronic states of this MOF on hBN can be tuned, inducing controllable metal-to-insulator transitions in this hybrid 2D material. Our findings pave the way for nanoelectronics and spintronics technologies based on 2D MOFs and on electrostatic control of quantum phases therein.

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ABSTRACTS

A new rechargeable high-temperature all-solid-state iron-air battery for efficient energy storage

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Abstract: High-temperature all-solid-state iron-air batteries are emerging as a promising rechargeable battery technology owing to their environmental benignity, high energy density, and outstanding safety. Their operation involves oxygen redox reactions at air electrode, oxygen ion diffusion inside solid electrolyte, and conversion reaction between solid Fe_2O_3 and FeO_x ($0 \leq x < 3.0$) at fuel electrode. Although great promise, the current performance is still far from satisfied due to low O^{2-} diffusion rate in Fe_2O_3 lattice, unstable fuel electrode morphology and poor stability of the fuel electrode-electrolyte interface during cycling, that result in low Fe-utilization, poor energy efficiency, and limited lifespan. Herein, we report a new iron-air battery that can operate at reduced temperature with high efficiency, high energy density and high power density. Exceptional longevity of 1600 cycles with a negligible capacity fading, a remarkable Fe-utilization rate of 75% ($1075 \text{ mAh g}_{\text{Fe}}^{-1}$), and an outstanding energy efficiency of 86% is reached. The main strategy that leads to the improved performance is mainly discussed. And the future optimization is proposed.

Engineering bioinspired fire-retardant coatings for general fire protection

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Main Fire-retardant coatings have demonstrated effective fire protection for building materials ranging from flammable rigid polyurethane foam, timber, and steel. However, limited efficiency and poor interface adhesion limit their real-world applications. Recently, we have developed a series of bio-inspired polymeric and ceramifiable organic-inorganic hybrid coatings. Upon exposure to flame, the coating exhibits a mechanically robust, structurally integral char layer on the substrates. With around 200-600 μm in thickness, such coating exhibits an ability to make polymer foam self-extinguish rapidly, a desired UL-94 V-0 rating; and to slow down the burning of solid wood, and to provide exceptional thermal protection for steel structures. This series of work provides a universal strategy for creating fire-retardant coatings for diverse fire protection applications.

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Solar Energy for Future Chemical Manufacture from A Catalysis Perspective

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Solar energy has long been the primary source sustaining life and driving natural processes across ecosystems on Earth.[1] In recent years, its role has expanded, emerging as a promising alternative to address the pressing challenges of the global energy crisis and climate change. This discussion will explore various opportunities for converting solar energy into sustainable fuels and valuable chemicals. By examining materials design, catalytic reactions, and process engineering, we can unlock innovative pathways for harnessing sunlight in new ways. [2,3] Additionally, the discussion will highlight how solar energy can serve as a cornerstone for the future of chemical manufacturing, potentially reducing carbon emissions and dependence on fossil fuels. This talk will also delve into the broader potential of solar energy, not only as a terrestrial solution but as a critical consideration for human endeavours in space. In this way, solar energy stands as a pivotal resource, both for our sustainable future on Earth and for exploring humanity's next frontier.

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Unveiling the material's photo/electrochemical properties correlated with its electronic structures

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Abstract: Structure (from atomic and electronic level)-performance correlation demonstrates the crucial impact of complex surface chemistry and nanostructure on photo/electrochemical performance, which is also a persistent barrier for rationally designing photo/electrode materials. To rational design materials for their superior photo/electrochemical properties can only rely on the unveiling of the correlation between their electronic structures' evolution along the testing processes. Therefore, from the electronic level to develop the spatial- and time-resolved light interaction technology can the photo/electrochemical reactions processes be deeply understood. Therefore, here I showcase several recent works about investigating the intrinsic properties of the materials correlated with their subtle micro-structure variation, including,

1. Through a combination of theoretical calculations and experiments, I recently revealed how water molecules drive moisture electric generators (MEGs) in three main ways: 1). Water molecules are absorbed on the material's surface and split into hydroxy groups and protons due to the material's polarizability and static electric potential. This process changes the electrochemical potential of the materials. 2). Protons from the water splitting act as charge carriers. 3). Hydrogen bonds in water molecules help drive these charge carriers between electrodes, maintaining the current flow.

The study shows that anatase TiO₂ materials can change output voltage based on differences in work function, influenced by surface adsorbed species and the material's crystal facets. This work clarifies the general working principle of MEGs.^[1]

2. The heterojunction approach enhances photoelectric current for reactions like hydrogen evolution by improving the separation of photogenerated electrons and holes through proper band alignment between two materials. Most research focuses on different bulk nanomaterials, but few examine crystal structure effects. I unveiled a new way to optimize band alignments in heterogeneous catalysts for better photoelectric properties by looking at polyheptazine-structured g-C₃N₄ and wurtzite CdS. It finds that higher annealing temperatures make CdS expose its (110) facets, forming an S-scheme heterojunction with g-C₃N₄. This junction speeds up electron-hole recombination and enhances their separation, improving photocatalytic hydrogen evolution reaction (HER) performance.^[2]
3. Ion transfer issues and chemical instability in Zn anodes cause dendrites and side reactions. I recently introduced a Bi/Bi₂O₃ hybrid interphase that: 1) Protects the interface to suppress side reactions. 2). Prevents dendrite formation by favorably dissociating Zn atomic clusters. The Zn@Bi/Bi₂O₃ cell achieves high plating capacity (1.88 Ah cm⁻² at 5 mA cm⁻²) and lasts over 300 hours at high current density. The Zn@Bi/Bi₂O₃||MnO₂ full-cell retains 86.7% capacity after 500 cycles at 1 A g⁻¹, outperforming most interphases. The scaled-up battery (6 V, 1 Ah) combined with a photovoltaic panel shows excellent energy storage and long output (12 h). This approach promises ultrastable Zn anodes and applications in other metal-based batteries.^[3]

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Harnessing the giant and switchable surface energy of liquid metals for robotics

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Gallium-based liquid metal alloys are a special type of material that is in the liquid state at (or near) room temperature. They are particularly attractive due to their unique combination of a fluidic and metallic body, together with their exceptionally large surface tension (>600 mN/m, 9 times of water).[1] As a fluid, liquid metals provide the best union of stretchability, deformability, and electrical conductivity among all soft materials. Leveraging the unique combination of fluidics and metallic properties allows the electrical control of interfacial tension of liquid metals, enabling the development of soft actuators. Such actuators are simple, highly responsive, highly controllable, and reversible, which has led to the creation of useful devices such as reconfigurable antennas, artificial muscles, electrical switches, and soft robots.[2-3]

This talk will highlight our recent advancements in liquid metal electromechanical systems (LMEMS), with a focus on pioneering applications in robotics. Specifically, we have developed capillary liquid metal muscles (CLMM), which harness the dramatic, switchable change in liquid metal interfacial tension to produce force and movement. We first explore the theory behind the muscle's operation, calculate its estimated force output based on capillary size, and optimize its design for maximum force and stroke. We then assess force changes at various frequencies, movement with different payloads, and the impact of various electrolytes on performance. The CLMM's force output and position during movement can be precisely controlled using feedback mechanisms. It exhibits the greatest pressure variation per volt among all liquid-based actuators, demonstrating its potential for a wide range of applications, particularly where low-voltage operation is critical. Overall, the CLMM represents an exciting new class of actuators with significant potential in soft robotics.

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Discovery of higher charge superconductivity beyond charge-2e Cooper pairs

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Despite of the various forms of superconductivity, conventional or unconventional, topologically trivial or nontrivial, the condensation of charge-2e Cooper pairs has remained the origin and character of all superconductivity, as described by the BCS theory. We report our experimental discoveries of the charge-4e and charge-6e superconductivity in ultrathin ring devices fabricated using the kagome superconductor CsV₃Sb₅ [1]. These new phase coherent states are discovered by the observation of the quantized magnetic flux in units of $h/4e$ and $h/6e$ in systematic magneto-transport measurements. Our observations provide direct experimental evidence for the existence of phase coherent paired quantum matter beyond the charge-2e superconductors, and provide ground work for exploring the physical properties of the charge-4e and charge-6e superconductivity as unprecedented phases of matter beyond the condensation of Cooper pairs described by the BCS theory.

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Nanofluidic Energy Storage

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

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

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Electrically controlled room temperature magnetic phase transition and ultrafast colossal magnetoresistance in van der Waals magnetic materials

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Two-dimensional magnetic material has attracted extensive interest as a material platform for the development of low-energy spintronic devices. It has become a pursuit to explore room temperature two-dimensional magnetic materials and achieve electrical control of their properties. Here, we report two recent results of electrically-tuned magnetic properties in two-dimensional materials. Firstly, the magnetism of a quasi-2D magnet $\text{Cr}_{1.2}\text{Te}_2$ was manipulated via a protonic gate with an electron doping concentration up to $3.8 \times 10^{21} \text{ cm}^{-3}$. We observed non-monotonic evolutions in both coercivity and anomalous Hall resistivity. Under increased electron doping, the coercivities and anomalous Hall effects (AHEs) vanished, indicating a doping-induced magnetic phase transition. This occurred up to room temperature. Based on theoretical calculation results, it is confirmed a gate-voltage controlled ferromagnetic/antiferromagnetic transition. Secondly, this report will introduce the research results on electrically control of colossal magnetoresistance (CMR) in magnetic van der Waals nanoflake $\text{Mn}_3\text{Si}_2\text{Te}_6$. We have achieved ultra-low ($<5 \text{ A/cm}^2$) current control of the CMR effect and high-speed ($<50 \text{ }\mu\text{s}$) gate voltage control of high and low resistance states in this system. This phenomenon is originated from the spin orbit interaction of $\text{Mn}_3\text{Si}_2\text{Te}_6$. The current can induce spin polarization of itinerant electrons, and hence apply spin orbit torque to local spins, and change the magnetization direction of Mn atoms, achieving current control of CMR.

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Integrating perovskite oxides and layered materials towards future electronics

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When artificially integrating the naturally incompatible atomic structures, crystallographic orientations and physical functionalities, the interplays at the interfaces induce unexpected functionalities, which is beneficial to future electronics in the aspect of manipulation, functionalization and utilization [1]. However, realizing unrestricted heterogeneous integration and their electronic applications is extremely challenging, because of the technical restrictions of fabrication and the unwanted reduction of interface quality. The challenges are particularly severe in the heterogeneous integration of oxides with either other emerging materials or existing Si technologies, because of the incompatible growth dynamics and large lattice mismatch.

In this talk, I will discuss our recent exploration of functional electronic devices based on the heterogeneous integration of perovskite oxide films. First, I will provide a brief overview of the emergent functionalities in oxide heterostructures and approaches to heterogeneously integrating the perovskite oxides. Then, I will discuss on experimental results of two related electronic applications based on the heterogeneously integrated structures consisting of perovskite oxide membranes and layered two-dimensional materials, namely energy-efficient transistors using SrTiO₃ [2] and multifunctional devices using Sr-doped LaMnO₃ [3]. A summary will be provided at the end.

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Dipole Moment Tuning in Semiconductor Photoelectrodes

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

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A density-matrix renormalization group algorithm for non-hermitian physics

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A density-matrix renormalization group (DMRG) algorithm is proposed to deal with non-hermitian many-body systems with a biorthonormal-block representation (bbDMRG), in which a structured low-rank approximation to a non-hermitian reduced density matrix is necessarily made to satisfy the prerequisite on the biorthonormality of the renormalization transformation. Subsequently, a redundancy assigned to those saved blocks of reduced density matrix is exploited to reduce a condition number for both left and right transform matrices, which practically ensure the numerical stability of the renormalization procedure. The bbDMRG is successfully applied to an interacting fermionic Su–Schrieffer–Heeger model with imposing non-hermitian to the kinetic energy and various boundary conditions, for which a ground-state phase diagram is obtained to show fascinating phenomenon caused by the interaction and the non-hermitian as well.

Pathways to long-term stable perovskite solar cells

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Long-term stability remains a significant challenge in the development of perovskite solar cells (PSCs). In this presentation, I will explore novel strategies aimed at enhancing the stability of PSCs [1-5]. These approaches encompass various aspects including phase stability, ultraviolet stability, thermal stability, and more. Through a comprehensive discussion, I will discuss the potential mechanisms underlying the instabilities encountered in PSCs and propose corresponding solutions (Fig. 1). Our findings offer promising avenues towards achieving durable and commercially viable PSCs, contributing to the advancement of renewable energy technologies.

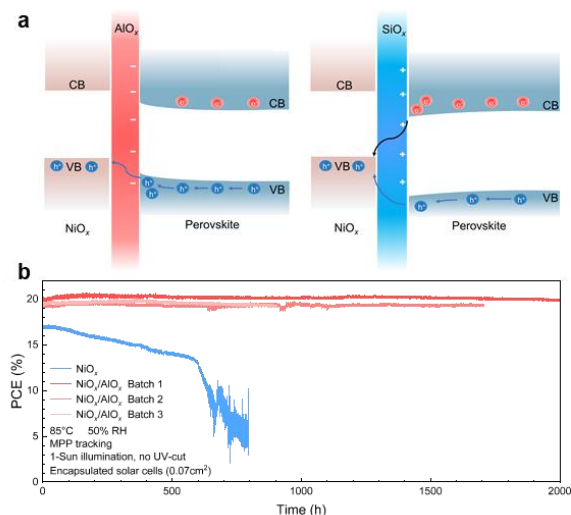


Fig.1 | Fixed charges at perovskite/NiO_x heterojunctions. **a**, Schematic illustrations of the electronic structure and carrier distribution in conduction and valence bands (CB, VB) for perovskite/NiO_x heterojunctions when (left) an AlO_x interlayer or (right) a SiO_x interlayer is included. Hole transport (blue arrow) occurs in both cases, but the fixed negative charges of the AlO_x interlayer reduce electron–hole recombination (black arrow) and the fixed positive charges of the SiO_x interlayer do not. **b**, The AlO_x-interlayered devices show long-term operational stability, maintaining photovoltaic cell efficiency (PCE) when aged at 85 °C and 50 % relative humidity under one sun illumination.

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Novel three-dimensional Fermi surface and electron-correlation-induced charge density wave in FeGe

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As the first magnetic kagome material to exhibit the charge density wave (CDW) order, FeGe has attracted much attention in recent studies. All the theoretically calculated phonon frequencies in FeGe remain positive. We perform a comprehensive study through first-principles calculations and symmetry analysis. We find that reasonable Heisenberg interactions and magnetic anisotropy cannot explain the double cone magnetic transition, and the DM interactions can result in this small magnetic cone angle. Based on the experimental 2X2X2 supercell, we thus explore the subgroups of the parent phase. Group theoretical analysis reveals that there are 68 different distortions, and only four of them without inversion and mirror symmetry thus can explain the low temperature magnetic structure. We also find that the maximum of nesting function is at K point instead of M point. Considering the effect of local Coulomb interaction, we reveal that the Fermi level eigenstates nested by vector K are mainly distributed from unequal sublattice occupancy, thus the instability at K point is significantly suppressed. Meanwhile, the wave functions nested by vector M have many ingredients located at the same Fe site, thus the instability at M point is enhanced. This indicates that the electron correlation, rather than electron-phonon interaction, plays a key role in the CDW transition at M point.

Tunable many-body interactions in bulk and edge of the 2D topological excitonic insulator WTe₂

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Coulomb interactions among electrons and holes in 2D semimetals with overlapping valence and conduction bands can give rise to a correlated insulating ground state via exciton formation and condensation – an *excitonic insulator*. One materials platform in which such excitonic insulating state uniquely combines with non-trivial band topology are atomic monolayers of tungsten ditelluride (WTe₂) [1-4], in which a *2D topological excitonic insulator* (2D TEI) forms.

From scanning probe spectroscopy down to 4.2K [3], we show that the 2D TEI state in WTe₂ is susceptible to a gate-tunable quantum phase transition – evident from an abrupt collapse of its 2D bulk energy gap upon ambipolar field-effect doping.

Impossible to explain from a single-particle picture, the quantum phase transition provides direct evidence of strong electronic correlations in the WTe₂ 2D bulk, stabilizing the topological gap at low doping. The 1D topological edge state, on the other hand, prevails across the phase transition harbouring a tunable helical Tomonaga-Luttinger Liquid (TLL) in the strongly coupling limit [4]. Field-effect tunability of a 2D Topological Excitonic Insulator (TEI) into either *n*- and *p*-type semimetals may promise novel handles of control over non-trivial 2D superconductivity with excitonic pairing.

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Phase Engineering using 2D Heterostructures & 2D MOF formation

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I will talk about two of our current projects on 2D materials. I will introduce our surface science lab and various 2D projects done. In the first current project, we report a phase-selective inplane heteroepitaxial method to grow semiconducting H-phase CrSe₂ (Nat. Comm. 2024). The lattice-matched MoSe₂ nanoribbons are utilized as the in-plane heteroepitaxial template to seed the growth of H-phase CrSe₂ with the formation of MoSe₂- CrSe₂ heterostructures. Scanning tunneling microscopy and non-contact atomic force microscopy studies reveal the atomically sharp heterostructure interfaces and the characteristic defects of mirror twin boundaries emerging in the H-phase CrSe₂ monolayers. Second, I will report a study of a conformationally flexible precursor 2,4,6-tris(3-bromophenyl)-1,3,5-triazine (mTBPT) on Cu(111) comprising a random phase of C3h and Cs conformers (Nat. Comm. 2024). At low coverage (0.01 ML) selenium (Se) doping, we achieved the selectivity of the C3h conformer and improved the nanopore structural homogeneity. Through the combination of high-resolution scanning tunneling microscopy, non-contact atomic force microscopy and density functional theory calculations, we explored the formation of the conformationally flexible mTBPT on Cu(111).

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Sustainable catalytic biorefining: Challenges and opportunities for catalyst design

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Concerns over dwindling oil reserves, CO₂ emissions from fossil fuel sources and associated climate change is driving the need for renewable energy. To keep the mean global temperature rise <1.5 °C, a large proportion of crude oil, gas and coal reserves are unavailable for energy use [i]. Biomass, derived from agricultural and forestry residues, or non-food sources of triglycerides is a sustainable source of carbon for low-cost solutions to transportation fuels and organic chemicals. Akin to petroleum refining, biorefining will integrate biomass conversion processes to produce fuels, power, and chemicals, thereby increasing the economic viability of bio-derived processes. [ii]. The drive for a ‘zero waste economy’ also encourages a circular approach to valorize waste feedstocks.

In contrast to fossil derived hydrocarbons, that generally require selective oxidation for chemical production, highly functional bio-derived molecules will require selective deoxygenation to their target products. Such transformations may involve cascade reactions, where multicomponent catalysts containing tunable acid or base sites may act in concert with metallic sites or cooperatively to promote sequential dehydration or condensation steps and metal catalyzed hydrogenation or oxidation steps. This presentation will discuss innovations in catalyst/process design required to overcome the scientific and engineering barriers to the economic production of low carbon fuels and chemicals from sustainable feedstocks. Case studies will explore nanoengineering of bifunctional catalysts for upgrading of bio-oils to fuels, [iii,^{iv}] and the production of platform chemicals and fuel precursors from waste derived sugars [v, vi].

Navigate the Chemical Space of Organic Cations in Hybrid Perovskites

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As an emerging class of light-responsive semiconductors, hybrid organo-metal perovskites seamlessly marry the characteristics of organic and inorganic materials, offering a new fertile playground to advance solution processing and to explore light-matter interaction. They have been studied by materials scientists for more than a century, but in the past decade, perovskites have attracted a new wave of intense interest due to their extraordinary photovoltaic properties. The hybrid characteristics of organometallic perovskites bring a unique combination of physical properties, while the strong correlation of composition/structure/function in these frontier materials exposes us to new challenges with unprecedented complexity. Here, I will talk about our recent efforts to adapt machine-learning and high-throughput approaches to navigate the vast chemical space of organic cations in hybrid perovskites. The generative method accelerates the discovery and design of new materials, achieving precise control of the energy band structure of two-dimensional hybrid perovskites. Furthermore, the intricate interactions of organic molecules and inorganic framework of hybrid perovskites allow effective multi-site passivation of the perovskite surfaces, leading to high photovoltaic performance.

Solvation and Interfacial Chemistry in Ionic Liquid Based Electrolytes toward Rechargeable Lithium-metal Batteries

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Rechargeable lithium metal batteries (LMBs) are highly promising technologies for high-energy-density storage systems due to the low electrochemical potential and high theoretical capacity of lithium metal anodes (LMAs). Nevertheless, traditional carbonate-based and ether-based electrolytes tend to undergo uncontrolled side reactions with LMAs and high-energy cathode materials, leading to severe lithium dendrite growth and electrolyte depletion. A practical approach to overcoming these challenges is to use novel electrolyte systems to build a stable and robust electrode/electrolyte interface (EEI) in LMBs, including solid electrolyte interphase (SEI) and cathode electrolyte interphase (CEI).^[1]

We have found unlike conventional electrolyte solvents, ionic liquids (ILs) are room-temperature molten salts composed of anions and cations. They exhibit ultra-low volatility, high ionic conductivity, excellent thermal stability, low flammability, and a wide electrochemical window.^[2] These properties make liquid IL electrolytes (ILEs) and solid polymerized ILEs (PILEs) highly promising for enhancing the cycling stability, energy density, lifespan, and safety of LMBs.^[3]

Herein, based on our extensive previous research and the latest literature, we systematically summarize three primary applications of ILs in LMB electrolytes. First, ILs serve as the main solvent in liquid electrolytes. Second, PILs are applied as solid-state electrolytes for solid-state batteries. Third, ILs are used in targeted electrode/electrolyte interface treatments, such as electrolyte additives, interfacial wetting agents, and ex-situ treatments of electrodes. Research on ILs and PILs as LMB electrolytes remains in its early stages, with limited understanding of key aspects like electrolyte solvation structures and the dynamic evolution of interfacial chemistry. Lastly, we proposed a design for high-safety, high-performance solid-state/semi-solid-state batteries based on electrode solidification. This design utilizes PILs to achieve electrode solidification and develops nonflammable, safe, specialized IL electrolytes, offering promising potential for IL applications and solid-state battery advancements.

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Metal-halide Perovskites for Light Emission Applications

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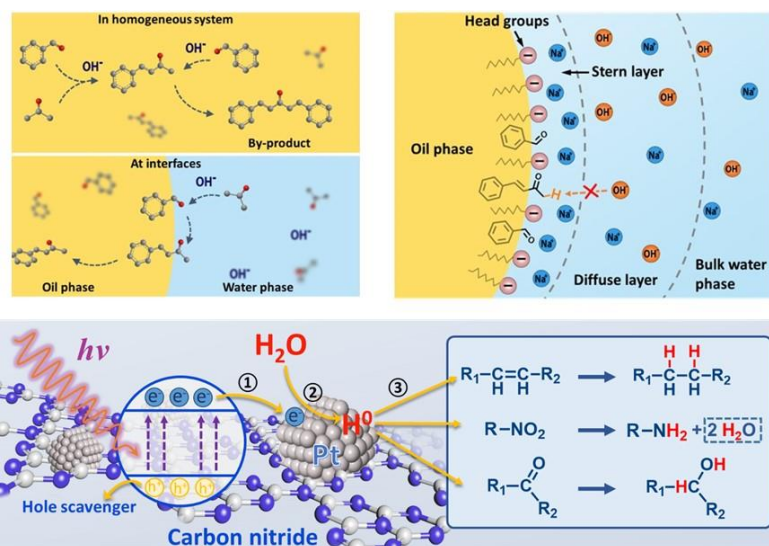
The development of high-efficiency, stable and low-cost luminescent materials and devices is one of the most effective ways to achieve efficient use of energy, and is an important guarantee for our country's transition to a low-carbon economy. Metal-halide perovskites possess the advantages of both inorganic and organic materials, and have great potential for low-cost, large-area, flexible display and lighting applications. The core of the work of perovskite light-emitting devices is the carrier dynamics of the functional layer under the driving of electric/optical field. Therefore, the detection, understanding and manipulation the carrier dynamics in perovskite by tailoring the materials' dimensionality and size are the key scientific issues in this field. In this report, we will introduce our recent discoveries on the excellent luminescent properties of metal-halide perovskites, the detection and regulation of carrier dynamics, research works on performance optimization of light-emitting devices and development of new luminescent applications.

Liquids Interfacial Catalysis and Photocatalysis with New Protocols

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Abstract: Catalysis plays a critical role in molecular transformation and chemical processing. In the past few years: (1) We have developed catalytic processes at the liquid-liquid interfaces in emulsion system to restrain the reaction paths, demonstrating higher atomic efficiency and better selectivity compared to conventional heterogenous/homogenous counterparts [1-3]. (2) Solar energy is more sustainable than any other energy source. We used the photocatalysis technique for hydrogenation reactions with water as the proton source, instead of traditional hydrogen gas or organic molecules [4-5]. (3) A triphase photocatalytic system to generate H_2O_2 at the air-liquid-solid joint interfaces is developed, which allows for rapid transport of oxygen from the air to the reaction interface, overcoming the low solubility and slow diffusion of oxygen in the water and reaching a benchmark H_2O_2 generation rate.



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Strategies enabling highly efficient interfacial solar evaporation

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Interfacial solar evaporation (ISE) is a green and sustainable technology to accelerate water evaporation using solar light as the sole energy source. Due to its unique advantages, ISE has shown great potential in wide range of applications including seawater desalination, industry wastewater treatment, and soil remediation [1,2]. During the last several years, great effort has been devoted to developing efficient photothermal materials and solar evaporators to improve energy efficiency and evaporation rate [3-5]. In addition, rational energy management is also crucial for significantly improving the energy efficiency of ISE [6]. In this presentation, recently developed strategies for highly efficient solar evaporation will be introduced.

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Room-temperature antisymmetric magnetoresistance and skyrmionic spin textures in van der Waals ferromagnet Fe₃GaTe₂ nanosheets

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Van der Waals (vdW) ferromagnetic materials have emerged as a promising platform for the development of 2D spintronic devices. However, studies to date are restricted to vdW ferromagnetic materials with low Curie temperature (T_c) and small magnetic anisotropy. Here, a chemical vapor transport method is developed to synthesize a high-quality room-temperature ferromagnet, Fe₃GaTe₂ (c-Fe₃GaTe₂), which boasts a high $T_c = 356$ K and large perpendicular magnetic anisotropy. Due to the planar symmetry breaking, an unconventional room-temperature antisymmetric magnetoresistance (MR) is first observed in c-Fe₃GaTe₂ devices with step features, manifesting as three distinctive states of high, intermediate, and low resistance with the sweeping magnetic field. Moreover, the modulation of the antisymmetric MR is demonstrated by controlling the height of the surface steps [1]. In addition, skyrmions of distinct topological charges are artificially introduced and engineered using magnetic force microscopy. The skyrmion lattice with opposite topological charges ($S = \pm 1$) can be tailored at the target regions to form topological skyrmion junctions (TSJs) with specific configurations. The delicate interplay of TSJs and spin-polarized device current were finally investigated via the *in-situ* transport measurements, alongside the topological stability of TSJs [2]. Our work provides new routes not only to achieve room-temperature 2D spintronic devices such as magnetic random storage and logic devices by utilizing the room-temperature antisymmetric MR, but also presents prospects for Fe₃GaTe₂-based heterostructures with the engineered topological spin textures.

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Investigation of chemo-mechanical failure in rechargeable batteries

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Current lithium-ion (Li-ion) batteries do not satisfy the increasing demands of portable electronic devices and electric vehicles, due to low energy densities, safety issues and high cost. High-capacity electrode materials are needed, and researchers have made significant progress over recent years. However, integrating these materials into practical cells has lagged due to several technical challenges. For example, volume expansion of active particles and mechanical stresses generated during cycling may cause cracking and interfacial debonding. Up to now, a fundamental understanding of the chemo-mechanical failure during charging/discharging cycles is still lacking. In this presentation, we like to report our recent work on investigation of material failure and degradation in different rechargeable batteries via electrochemical and material characterization, mechanical testing, and atomistic modeling. Firstly, we discuss the evolution of microstructure, phase composition, particle size and mechanical stress in Si anode in Li-ion batteries during charging/discharging cycles and relevant strategies to overcome cracking and pulverization of Si particles. Then, our recent activities in development of different rechargeable batteries will be briefly introduced.

Understanding and Improving stability of hybrid perovskite

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Organic-inorganic hybrid perovskites have emerged in recent years as one of the most promising materials for solution-processed electronics and optoelectronics including solar cells, light-emitting diodes (LED) and field-effect transistors (FET). There is an active exploration of different organic molecules contribution to the materials behaviour and also the use of novel interfacial layer and their functions to improve the performance of the devices. The key to the successful implementation of any materials systems depends very much on the understanding of degradation mechanism and the how facile is the methodology for the improvement. In this presentation, it will be shown on how the understanding of the materials can lead to simple solution with good outcome.

As it is widely known, the lack of long-term stability of hybrid perovskite materials remains an impediment to widespread implementation. A unified understanding of the complexity describing the degradation of these type of materials is absent and in this work one common hybrid perovskite material - methylammonium lead iodide (MAPI) is used as a vehicle to show how a unified understanding can be achieved using a complementary characterization techniques. This work uses low-dose in-situ electron microscopes and time-resolved photoluminescence (TRPL) to demonstrate that material loss is initiated at the MAPI grain boundaries near the negative electrode interface where MA⁺ is reduced.

In solar cells application, there are two critical performance indicators – efficiency and stability. Two layers combination making up of three-dimensional (3D) perovskite capped with low-dimensional (LD) perovskites materials have shown be an effective strategy in resolving the compromise that we have to live with for hybrid perovskites – compromise between photovoltaic efficiency and operational stability. In the study, instead of the conventional LD capping layers containing Pb²⁺ or Sn²⁺, we showed that through a full precursor technology option, it is possible to access a wider cation library for these capping layers.(1) Through this method, high efficiency cells can be achieved.

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Barocaloric Materials – Cooling and Heat storage –Atomic Level Understanding with Neutrons

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Refrigeration is crucial for modern society, enabling food storage and air conditioning, and it accounts for about 30 percent of the world's electricity consumption. However, current refrigeration technology, which primarily relies on the conventional vapor compression cycle, raises significant environmental concerns due to the substantial release of greenhouse gases each year. As a promising alternative, refrigeration technologies based on solid-state caloric effects have been garnering attention for several decades. The search for novel materials that exhibit large isothermal entropy changes during phase transitions induced by a small external field is central to the study of solid-state caloric effects. Understanding the mechanism behind these large caloric effects and the associated phase transitions is fundamentally important.

In this presentation, I will discuss how inelastic neutron scattering and quasi-elastic neutron scattering can provide atomic-level insights into the mechanisms responsible for the colossal barocaloric effects (CBCEs) (large cooling effects induced by pressure) and the inverse barocaloric effect (thermal battery for heat storage) observed in plastic crystals [1-4].

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An overview of digital twin in Australian aerospace manufacturing

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This paper provides an overview of recent advancements in digital twin (DT) technology applied to composite components in the aerospace sector, with a focus on integrating DT with the digital thread concept. The first objective is to explore the evolution and application of digital twin technology, highlighting its potential to improve operational efficiency, reduce waste, and enhance product quality. Despite the progress in DT for individual components, the integration through a digital thread, a holistic framework, connecting all system components throughout their lifecycle remains undeveloped. The absence of a robust digital thread limits the full potential of DT, which could otherwise enable predictive maintenance, optimisation, and more efficient decision-making. The second objective focuses on reviewing the current implementation of the digital thread for aerospace composites. Despite the proven effectiveness of the digital thread system, it suffers from inefficiencies in the quality control cycle. These inefficiencies lead to substantial waste due to over-engineering, additional testing and inspections, and excessive scheduled maintenance. The paper explores use cases demonstrating the benefits of a well-implemented digital thread while identifying areas where its potential remains unexploited. The third objective proposes a roadmap for improving digital thread integration, emphasising comprehensive health monitoring across a component's lifecycle. It identifies key gaps in current methodologies and offers recommendations for improved digital thread implementation to enhance efficiency, accuracy, and overall effectiveness in aerospace manufacturing. These improvements aim to enhance design, manufacturing, and supply chain management, contributing to broader industry objectives such as achieving carbon-neutral aviation in 2050.

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Biomass-Derived Functional Materials for Energy Storage and Management

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Agricultural biomass, such as sugarcane bagasse and rice husk, is an abundant and renewable bioresource for producing fuels and chemicals. However, high production costs and low product values currently hinder commercialisation efforts. Biorefining agricultural biomass into multiple products, including high-value functional materials, has the potential to significantly improve overall process economics.

Professor Zhanying Zhang and his team at Queensland University of Technology (QUT) are developing multiproduct biorefinery processes and technologies to convert agricultural biomass into fermentable sugars, cellulose and nanocellulose materials, lignin nanoparticles, lignin-derived carbon materials, and biosilica nanoparticles for various applications. Their multiproduct biorefineries are based on advanced biomass pretreatment technologies, which are essential for effective biomass deconstruction, separation, and control of biomass component properties. In this presentation, Professor Zhang will summarise the group's research achievements in multiproduct biorefineries, focusing on the development of cellulose nanocrystal (CNC)-derived photonic films for solvent detection and radiative cooling, as well as lignin-derived hard carbon for sodium-ion battery anode applications.

Phase Engineering of Nanomaterials (PEN)

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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. By using gas-solid reactions, metastable 1T'-phase group VI transition metal dichalcogenides (TMDs), *e.g.*, WS₂, WSe₂, MoS₂, MoSe₂, WS₂xSe_{2(1-x)} and MoS₂xSe_{2(1-x)}, have been prepared. Impressively, the 1T'-MoS₂-supported single-atomically dispersed Pt (s-Pt) atoms with Pt loading up to 10 wt% exhibit superior performance in hydrogen evolution reaction. Importantly, 1T'-TMD monolayers can be stabilized on 4H-Au nanowires, which can be used for ultrasensitive SERS detection. 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.

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Peptide-Based Nanoemulsions and Nanocapsules: Versatile Platforms for Advanced Applications

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Abstract:

Peptides are versatile biomolecules with unique structural and functional properties, making them ideal candidates for modular design in nanomaterial applications. Their inherent biocompatibility and ability to be engineered for specific interactions allow for the creation of peptide-based nanoemulsions and nanocapsules with advanced functionalities. By leveraging the surface activity of peptides, they can be tailored to form stable nanoemulsions, which exhibit stimuli-responsive behavior, opening new avenues for delivery applications. Furthermore, peptides can be designed with dual functionality, possessing both surface activity and the ability to facilitate biosilicification, thereby enabling the formation of nanocapsules with core-shell structures. These nanostructures provide a flexible platform for encapsulating active agents within the core while allowing surface modification with functional groups or targeted molecules for drug delivery and cell therapies. Such peptide-based nanomaterials hold significant promise in drug delivery and cell therapy applications, offering innovative solutions for biomedical applications, and improved bioavailability. This talk introduces the design, synthesis, and broad potential applications of peptide-based nanoemulsions and nanocapsules, highlighting their role in advancing next-generation biomedical applications.

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Innovation of Seawater Electrolysis

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Using renewable energy to produce green chemicals and fuels via electrolysis is economic and environmentally beneficial for Australia. For example, in many water electrolyzer technologies for H₂ generation, the proton source is from the water. Because of use of highly active precious metal catalysts Pt and Ir, there is a strict requirement for quality of the water feedstock, e.g. ultrapure DI water. Increasing demand for H₂ to partially, or totally, replace fossil energy will significantly exacerbate present scarcity of limited freshwater. Seawater is an (almost) unlimited resource and a natural feedstock for H₂. This is practical for geographical regions with long coastlines and abundant sunlight, but freshwater is actually scarce in Australia. Because of salt (Na⁺, Cl⁻) and minor ions/cations (SO₄²⁻, CO₃²⁻, Mg²⁺ and Ca²⁺), it is necessary to treat seawater to a level of purity for conventional electrolyzer including desalination and deionization. Here we identified two representative reactions, namely, 1) direct seawater splitting to H₂ at cathode and, 2) natural chloride promoted C₂H₄ electrooxidation to 2-chloroethanol at anode, to demonstrate the concept of direct seawater-based electrocatalysis. The newly developed process – using natural seawater instead of purified water as feedstock – enables new concepts in electrocatalysis fundamentals, electrode materials design, and electrolyzer technology.

Optimising 2D Formamidinium Perovskites for Stable and Efficient Solar Cells

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Perovskite solar cells (PSCs) have made remarkable strides in achieving high power conversion efficiency, but their commercialization is still challenged by stability issues. Formamidinium (FA)-based two-dimensional (2D) perovskites have emerged as highly promising candidates due to the outstanding optoelectronic characteristics exhibited by inherent FA-based perovskites and enhanced environmental stability provided by 2D structures. The efficiency and stability of FA-based 2D PSCs are still relatively low.

In the first work using one-step deposition method. We tuned the Pb-I octahedral twisting and lattice distortion by organic spacer cation engineering to stabilise the FA-based 2D perovskite lattice. We further modulated the crystallization kinetics with a molecular-type Selenourea (SU) additive to inhibit the in-plane growth of quantum wells in 2D perovskites. The optimized FA-based 2D PSCs achieved a record-high power conversion efficiency (PCE) of 20.03% and exhibited less than 1% efficiency degradation after operating at maximum power point for 1000 hours.[1]

In the second work, we developed an additive-stabilized spacer-cation-preponed two-step deposition method to achieve the out-of-plane orientation and grain sizes larger than 5 μm in 2D perovskites. The optimized 2D PSCs achieved a high PCE of 21.16% and a short-circuit current of 23.71 mA cm^{-2} , among the highest in 2D PSCs. The PSCs demonstrate remarkable stability, with a PCE decrease of less than 5% after exposure to 65 $\pm$ 10% humidity for 1100 hours, operation at 85°C for 1077 hours, or continuous illumination for 1045 hours.[2]

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New Rashba Physics and Prototypical Device Applications

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The Rashba effect is one iconic manifestation of spin-orbit coupling in crystal systems with broken inversion symmetry. In recent years, photoemission experiments have convincingly revealed that the seminal linear-order Rashba theory oversimplifies the complex hierarchic spin splitting band structures, reinvigorating the theoretical explorations of new Rashba mechanisms such as k -cubic contributions and type-II Rashba with hidden spin polarizations. In this talk, we will overview our recent works on new Rashba physics in the 2D limit and related device prototypes based on these findings, including: gate-tunable Rashba valleys and quantum Hall effects in centrosymmetric black arsenic electronic gases; and hidden spin activations and anomalous magnetoresistance in type-II Rashba systems, which provide an amazing material platform for developing spintronics and highly efficient room-temperature planar Hall sensors.

Electrochemical Engineering and Direct Ink Writing 3D Printing: Cost-Effective Production of 2D Nanomaterials and their Bespoke Assemblies

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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 NH₄F 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 incorporation of C12E9 offers amphiphilicity to the MXene flakes and produces a 3D interlinked network of the MXene flakes. 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.

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ABSTRACTS

High performance anode materials for direct methane fuel cells

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The efficiency of solid oxide fuel cells (SOFCs) can be over 60%. The high operating temperature of SOFCs makes it possible for them to directly use hydrocarbons such as methane as the fuel without the need of pre-reforming process. Traditionally, Ni-based cermets are used as the anodes of SOFCs because of their high catalytic activity and electronic conductivity. Unfortunately, the quick degradation of Ni-based anodes by detrimental carbon accumulation significantly retards the progressing of direct methane SOFCs. This presentation will introduce the research on the development of high performance anodes for direct methane fuel cells in our group.

2D metal oxide nanostructures for green hydrogen production

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Hydrogen energy has been regarded as one promising alternative to displace current fossil energy resources by its high energy value and zero CO₂ emission to address the increasing environment and energy crises. Especially, electrochemical water splitting hydrogen production is expected to be the most feasible approach with a good balance of cost and efficiency, in which electrocatalysts are the most critical component and govern the conversion cost and energy consumption. Therefore, the search of affordable catalysts with comparable catalytic performance to replace with the current expensive noble-metal-based catalysts in real water conditions is an urgent priority. In this presentation, inspired by the salient properties of 2D materials, promising 2D metal oxide-based electrocatalysts for electrochemical hydrogen production through mechanism understandings and performance upgrades will be presented. It is expected that this presentation will provide some insights in designing low-cost but efficient non-noble-metal catalysts for reaching affordable green hydrogen energy.

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INVITED PRESENTATION

Before Digging Deep, Collect the Treasures from the Surface

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Highlights from combined experimental and theoretical research on battery surfaces are presented. Nano structural characterization and associated properties provide evidence of the important role played by surfaces for enhancing key battery properties of material particles.

Our focus on battery surfaces started from identification of a structural differentiation between the surfaces and cores of battery particles [1-3]. A variety of laboratory surface techniques such as Raman and X-ray photoemission spectroscopy, and synchrotron experiments confirmed this differentiation. The effect of surfaces on reflectance spectra, used to determine electronic band gaps after conversion to absorption, provided a consistent explanation of variable results reported in the literature. An improved selection of pseudopotentials for Density Functional Theory (DFT) calculations was also utilized, resulting in better match(es) between calculated and experimentally measured band gap values.

The surfaces and core of particles can be well approximated by semiconductor junction-like effects [4], where favorable interface(s) and electronic band alignments can be designed to enhance performance. Phosphate coatings on Lithium- and Manganese-rich Nickel, Cobalt and Manganese (NMC) oxide materials were designed along these principles for electronic band structure alignment with substantial improvements to surface stability, rate capability and cycle life demonstrated [5-7].

Enhancements of surface properties for commercial formulations of Nickel-rich NMC materials were also attributed to modifications on the surfaces from ppm levels of Ca impurity segregation. Such results provide potential commercial advantages by reducing purification costs for raw materials and by self-producing modified surface nano structures that need not require use of surface coatings post particle manufacture. Similar surface enhancements have been demonstrated for graphitic anode materials [8].

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Phase engineering by ions-modulation for durable oxygen evolution

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As is well known, the activity of the electrocatalytic oxygen evolution reaction (OER) mainly depends on the active sites of the electrocatalyst.^[1] In certain oxide electrocatalysts, high-valence metal sites (such as molybdenum oxide) are often not the true active centers for electrocatalytic reactions, primarily due to their poor intermediate adsorption behavior.^[2] As proof of concept, we can select molybdenum oxide as a representative model catalyst, where the intrinsic molybdenum sites are not favorable active centers. By introducing anion doping, such as N/P/B regulation through defect engineering and phase engineering, the inactive molybdenum sites can be regenerated into synergistic active centers that promote OER. Through a comprehensive comparison, it was found that the OER performance of oxide catalysts is highly correlated with phosphorus sites and molybdenum/oxygen defects. Additionally, B/N doping can induce phase changes in molybdenum oxide that are more favorable for OER. This work is expected to provide insights into enhancing electrocatalytic performance by activating inert metal sites on oxide catalysts to enrich metal active sites.

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High-performance Electronic Devices Enabled by Atomically Sharp Interface in van der Waals Heterostructures

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While the scaling of devices continues, to meet the increasing demands for high performance, silicon-based technology meets a key challenge of the unavoidable interfacial dangling bonds in ultrathin-body silicon, which causes substantial degradation in device performance. It is thus an urgent need to seek atomically sharp interfaces and seamlessly integrate them into the device architecture. Among all candidates, emerging two-dimensional (2D) materials and their heterostructures represent ideal atomically flat in-plane surfaces potentially free from surface dangling bonds and are immune to short-channel effects that can allow effective electrostatic control and mechanical flexibility.

In this talk, I will demonstrate that by mechanical exfoliation and dry-transfer method, InSe/hBN/graphite van der Waals (vdWs) heterostructure with atomically sharp interface have been successfully achieved. This vdWs heterostructure can work as the unit of 2D field-effect transistor (FET), with electron mobility up to $1146 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ at room temperature and on/off ratio up to 10^{10} [1]. Furthermore, it can also work as the core component of the photodetector with a high on/off ratio of over 10^8 , high photoresponsivity up to 14250 AW^{-1} , and photodetectivity as high as 1.63×10^{13} Jones even at zero gate voltage due to the successful suppression of the dark current to 10^{-14} A [2]. When we placed it onto SiO_2/Si substrate, this heterostructure can work as a floating-gated FET, an elementary device of flash memory. Due to the improved interfacial coupling and atomically sharp interface, ultrahigh-speed operation with nanosecond write and read times that is limited by instrumentation response, extremely high extinction ratio of 10^{10} and a retention time of 10 year have been achieved [3,4].

All the above results highlight that van der Waals heterostructures offer a unique platform for next-generation high-performance electronic devices.

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ABSTRACTS

Making Patterned Single Defects in MoS₂ Thermally with the MoS₂/Au Moire Interface

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Normally, it is hard to regulate thermal defects precisely in their host lattice, due to stochastic nature of thermal activation. Here, we demonstrate a thermal annealing way to create patterned single sulfur vacancy (V_s) defects in monolayer molybdenum disulfide (MoS₂) with about 2 nanometer separations at sub-nanometer accuracy. Theoretically we reveal that the S-Au interface coupling reduces the energy barriers in forming V_s defects and that explains the overwhelming formation of interface V_s defects. We also discover a phonon regulation mechanism by the moiré interface that effectively condenses the Γ -point out-of-plane acoustic phonons of monolayer MoS₂ to its TOP moiré sites, which has been proposed to trigger the moiré-patterned thermal V_s formation. The high-throughput nanoscale patterned defects presented here may pave the way towards building scalable defect-based quantum systems.

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Engineering Metal Halide Perovskite Films for Photovoltaic Devices

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Metal halide perovskites have shown great promise for a broad range of applications due to their fascinating optical, chemical, physical and optoelectronic properties. A class example of perovskites' applications is photovoltaic (PV) devices, convert sunlight directly into electricity. Despite the great promise and advancements, the commercialization of this cutting-edge technology is limited due to the issues associated with the stability of perovskite in ambient conditions and heat. Engineering strategies such as additive engineering and surface passivation are promising approaches for not only improving the stability of perovskite solar cells, while also enhancing the PV performances. In this talk, I will present our recent work focused on engineering metal halide perovskite using O₂-inducing effect and surface passivation methods and their application in solar cells.

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Hard carbons influence of structure, pre sodiation and electrolyte choice

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Battery storage systems are a crucial element in achieving sustainable clean energy. Na-ion batteries represent the future in energy storage systems because of the wide availability and abundance of Na⁺ and because they require fewer critical minerals in their makeup. Unlike current state of the art lithium ion batteries, which require highly structured graphite as the anode, Na-ion perform best with carbon anodes which are non-graphitizable termed hard carbons. In recent times hard carbons from waste streams have gained some interest however despite the precursors choice some inherent limitations remain for hard carbons such as low initial columbic efficiency and rate capability limitations. In his talk we explore these limitations by examining the impact of electrolyte choice on performance and namely the solid electrolyte interphase, we explore approaches to pre sodiate the anode, as well synthesis new carbons by combining hard and soft carbons to create a heterostructure.

In this talk we explore how the choice of precursors, conversion process used, temperature, atmosphere, time, rate, electrolyte and pre sodiation influence electrochemical performance drawing some conclusions on the role of the solid electrolyte interphase and the bulk property sodium storage mechanism.

ABSTRACTS

High-performance MOD-derived REBCO superconducting coated conductors with thick REBaCuO films

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In the past decades, REBa₂Cu₃O_{7- δ} (REBCO; RE = Y, rare earth element) second-generation high-temperature superconducting coated conductors have been considered one of the most promising superconducting materials. Enhancing in-field flux pinning and increasing film thickness have always been the main research directions in various popular film preparation routes. The good solutions for these two problems in MOD-derived REBCO are the nanocrystal addition and the semi-growth strategies for flux pinning and thick film preparation respectively. Thanks to a low-cost, continuous MOD preparation line from **Shanghai Creative Superconductor Technologies Co., Ltd.**, with 3 - 4 μm thick MOD-derived REBCO tapes were stably fabricated to hundreds of meters with high self-field and in-field performances by combining the BaHfO₃ nanocrystal addition and the semi-growth. Our semi-growth method provides great potential for preparing much thicker MOD-derived REBCO films, which also promote the industrialization and the application of REBCO thick tapes.

Keywords: High-temperature superconductor, REBa₂Cu₃O_{7- δ} , artificial flux pinning, nanocrystal addition, in-field performance

Properties and Applications of Boron Nitride Nanosheets

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Hexagonal boron nitride (*h*-BN) is a layered material with a crystal structure similar to that of graphite. However, unlike graphite, *h*-BN is an insulator, featuring an indirect bandgap of approximately 6 eV. In recent years, *h*-BN has attracted considerable research attention due to its remarkable properties, such as excellent thermal conductivity and chemical stability. Boron nitride nanosheets (BNNSs), which are atomically thin forms of *h*-BN, not only preserve these outstanding characteristics but also demonstrate enhanced performance relative to their bulk counterparts because of their reduced thickness [1]. This presentation will explore the unique thickness-dependent properties of BNNSs, including their Raman signatures [2], distinct adsorption behavior [3], thermal conductivity [4-5], and thermal expansion coefficients [4,6]. We will also investigate the mechanisms underlying these atomic-scale thickness effects. Additionally, we will discuss various applications of BNNSs in surface-enhanced Raman spectroscopy [7], thermal management [8], and energy harvesting [9], emphasizing the practical implications of their unique properties.

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Fluorescence Brightness Enhancement in Nanodiamond Quantum Sensors – Correlative Photoluminescence and Transmission Electron Microscopy (TEMPL) Studies

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Fluorescent Nanodiamonds (FNDs), diamond particles containing atomic defect color-centers, draw widespread attention due to their exceptional optical and spin properties, which make them excellent candidates for room-temperature quantum sensing and biomedical diagnostic applications. However, it is now recognized that continued advances of FND applications mandate a precise understanding of the crystallographic environment around the defect centres as well as the surface properties of the particles themselves. These factors have been speculated to strongly affect their fluorescent brightness and optical stability. Moreover as most of the FND fabrication is a top-down process where larger diamond crystals are milled to desired nanometer size, FNDs generally have broad size distribution and irregular shapes and have shown to exhibit as large as 7 fold brightness variations for same nominal size. Hence, an understanding of the electronic structure of FND surfaces, and ultimately how to control them, becomes important for FND applications.

Conventionally optical microscopy and a range of spectroscopies including fluorescence microscopy, Raman and electron paramagnetic resonance (EPR) are valuable in measuring different types of color centers in diamond. However due to the wavelength limitation, the optical measurement methods generally have resolutions of ~hundreds of nm. In order to achieve better understanding of FND properties, transmission electron microscopy offers better resolution and capabilities to provide insights at atomic resolution. My group has been developing methods using electron energy loss spectroscopy (EELS) in a TEM to detect and locate color center related defects, and the surfaces structures of FNDs. In particular, our results demonstrate that locations of NV centers can be measured [1] at better than 1nm resolution [2]. In addition the generally poorer signal-to-noise of EELS is ultimately compensated by the highly localized (subnanometer) probe, which enables unambiguous spectroscopic data obtained directly from the FND surfaces. By directly correlating with the fluorescence microscopy map, our newly developed correlative TEM and fluorescence microscopy (TEMPL) demonstrates that the 3D shapes of FND have strong effect to their brightness up to 4 folds enhancement for FNDs < ~100 nm [3]. Such direct electron microscopy and spectroscopic data in being able to distinguish between competing effects within complex FND, is valuable in advancing FND production and applications. Please underline the Presenter's name and include the email address in the affiliation information below the authors' names.

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Stabilizing perovskite solar cells: from Pb-based to Pb-free

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The recent decade has witnessed the rapid increase in the power conversion efficiency of metal halide perovskite solar cells. Despite their success in achieving intriguing photovoltaic performance, the inferior stability of PSCs against external stimuli (e.g. moisture, oxygen, UV light) remains a critical hurdle for their further large-scale applications. Herein, we introduced surface chemistry [1-2] and interfacial engineering strategies [3-4] to stabilize the photoactive phase and simultaneously passivate surface defects of perovskites for optoelectronic applications. As a result, the fabricated lead-based perovskite solar cells showed improved power conversion efficiency and exceptional durability under operational conditions. The as-developed 2D-3D perovskite heterostructure is also applicable to induce oriented growth of high-quality tin-based perovskite thin films for efficient lead-free perovskite solar cells. Besides, the synthesized perovskite-metal organic framework composites showed excellent photoluminescence stability against water immersion for 10,000 hours, which can serve as a desirable encapsulation technique for perovskite optoelectronics in the future.

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Bifunctional binder for Shuttle free Aqueous Zinc Iodine Battery

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Aqueous zinc-iodine (Zn-I₂) batteries have attracted considerable research interest as an alternative energy storage system due to their high specific capacity, intrinsic safety, and low cost. However, the notorious shuttling effect of soluble polyiodides causes severe capacity loss and poor electrochemical reversibility, greatly restricting their practical usage. Herein, we report a bifunctional binder (LA133) with strong iodine-chemisorption capability for aqueous Zn-I₂ batteries to suppress the shuttling effect. From both calculation and experimental data, we revealed that the amide and carboxyl groups in LA133 binder can strongly bond to polyiodides, significantly immobilizing the iodine at the cathode side. Due to the strong iodine immobilization, the Zn-I₂ battery with LA133 binder shows less side reaction, slower hydrogen evolution, lesser Zn dendrite growth, and lower self-discharge. Consequently, the Zn-I₂ battery using LA133 binder obtains high specific capacity (202.8 mAh g⁻¹) with high iodine utilization efficiency (96.1%), and long cycling lifespan (2700 cycles). Even at the high mass loading of 8.07 mg cm⁻², the battery can still retain 83.3% of its initial capacity after 1000 cycles. This work opens a new avenue to address the shuttling challenge of Zn-I₂ batteries through bifunctional binder.

Biography:

Dr. Shi CHEN, graduated from National University of Singapore, Surface Science Lab at 2011. He worked as research fellow in Nanyang Technological University from 2012 to 2017. In 2017, he Joined IMRE as a scientist in characterization group. In 2018, he joined Institute of Applied Physics and Materials Engineering, University of Macau as an assistant professor. His research interests focus on materials interface, including perovskite materials and battery materials. He is interested in the in-situ and operando investigation of materials interface for battery materials.

Colloidal Synthesis of Photocatalytic Quantum Dots Heterostructure

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Colloidal synthesis using Ligand mediated surface engineering is a powerful approach to manifest the physical and chemical properties of quantum dots. [1,2] We present a colloidal synthesis method to attract high-quality carbon quantum dots with surface ligand-induced dual emission through a colloidal synthesis strategy. [3] 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, a new class of van der Waals heterojunction photocatalyst, which is synthesized by hot-injection method, whereby carbon dots (CDs) are grown in situ on ZnSe nanoplatelets (NPLs), i.e., metal chalcogenide quantum wells. [4] The resultant organic-inorganic hybrid nanoparticles, CD-NPLs, are able to perform methanol dehydrogenation with the occurrence of α -C-H splitting and C-C coupling. The novel CD-based organic-inorganic semiconductor heterojunction is poised to enable the discovery of a host of new nano-hybrid photocatalysts with full tunability in the band structure, charge transfer, and divergent surface chemistry for guiding photoredox pathways and accelerating reaction rates.

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Ultra-Small Gold Nanoparticle Particle Adsorption and Uptake is Directed by Particle Capping Agent

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Introduction: Nanomaterials are widely investigated, especially in many biological settings. This is due to their potential use as advanced nano-medicines and diagnostic technologies. In general, nanoparticle-based biotechnologies must interact with, and often cross, a cellular membrane to be useful; however, the dynamics of these interactions are still poorly characterized.

Aim: Combine advanced experimental and computational studies (see Fig 1) to investigate the interaction of ultra-small gold nanoparticles (AuNPs) with a variety of systematically varied capping agents at the interface of synthetic bio-membranes to determine the dynamic interaction of model systems at bio-membranes.

Methods: A combination of atomic force microscopy, light and energy scattering, and molecular dynamics simulations was used to study the fundamental behavior of the AuNPs at the bio-membrane-liquid interface. The systems of interest are models consisting of supported lipid bilayers (SLBs) and free-floating liposomes, which act as archetypal bio-membranes. The capping agent on the particles was purposefully varied. Liquid-phase and gel-phase biomembranes were used to systematically assess interactions.

Results: We investigated the behavior—dynamics, adsorption, translocation, and physical interactions—of a variety of AuNPs at the biomembrane interface. The techniques listed above are beginning to provide localized, nanoscale information on the dynamics and mechanisms governing the interactions of AuNPs and biomembranes.

Conclusion: The precise mechanism by which AuNPs adsorb to the bio-membrane is beginning to be elucidated, revealing several interesting behaviors: 1) initial adsorption, 2) nanoparticle incorporation and/or translocation, 3) particle-induced phase change, and 4) translocation of the particles. These interactions are of broad scientific and medical interest.

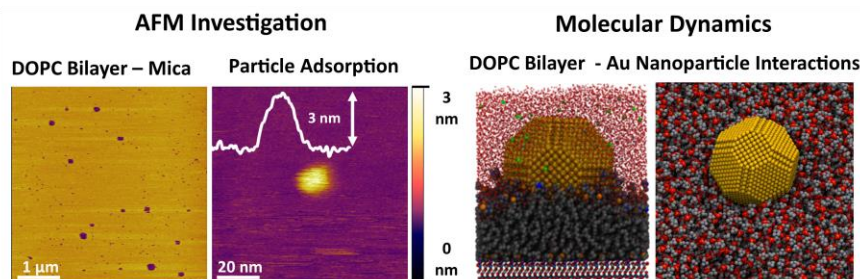


Figure 1. AFM and Molecular dynamics simulation investigation of the interaction of 5 nm AuNPs with a supported DOPC lipid bilayer formed at a mica surface.

Tailoring Polymer Brushes with Water and Light

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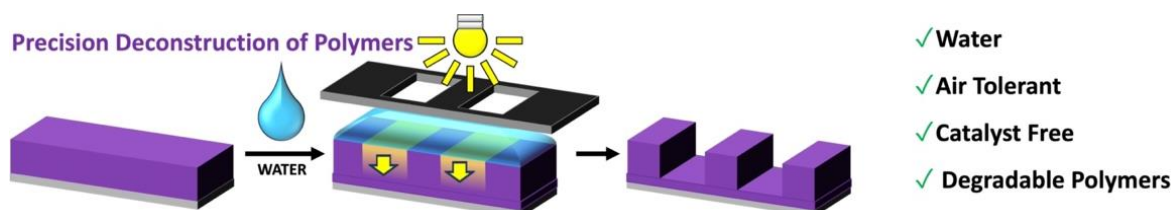
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Thin polymer films, known as polymer brushes, are a key technology for designing surfaces, with applications in biomedicine alone including biosensing, cell culture, regenerative medicine, and antibacterial coatings. The structuring of polymer brushes has the potential to precisely tailor the properties of these films for specific application requirements. However, extensive fabrication requirements can gatekeep this technology, preventing its application by potential end-users in various sectors. This presentation addresses these challenges by pioneering the first continuous subtractive patterning process.

We have recently shown that radical ring-opening polymerization of cyclic monomers can incorporate complex chemical structures from peptides^[1,2] to photocleavable cyclobutane rings^[3,4] into the polymer brush's main chain. Applied in surface induced radical ring-opening polymerization, photocleavable targets can be readily incorporated into the main chains of polymer brushes. After the initial fabrication, these brushes can be easily degraded with light, triggering photocleavage of the cyclobutane units. This not only enables continuous brush degradation for topographical patterning but also introduces alkene moieties that serve as points for further functionalization. Critically, the inherent photodegradability of the polymer brush eliminates the need for additional chemicals or catalysts. If the brush fragments are sufficiently water-soluble, the brush structuring can be carried out using nothing but water and light - in a process that can be done by anyone, anywhere.



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Exploring color center features in diamond nanostructures: a step towards advanced nano-photonics

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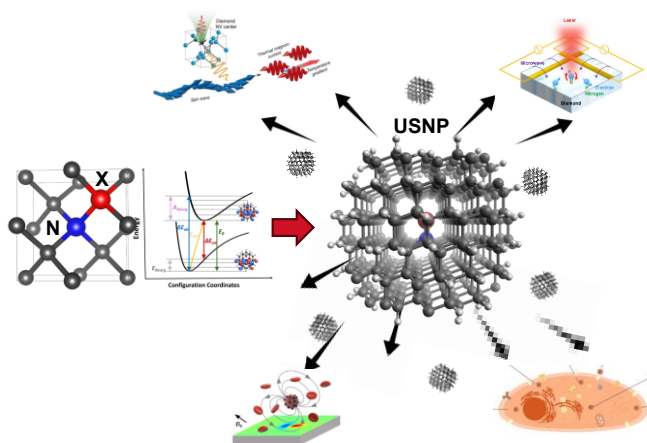
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Diamond Nitrogen Vacancy (NV) centres, with their stable spin configurations, high photostability, and long spin coherence times, are particularly promising for many technological applications, including biotechnology and quantum computing. However, current production techniques, such as detonation, high-pressure high-temperature processes, and chemical vapour deposition, have poor control over the size and morphology of the particles. Additionally, the charge state, primarily NV⁻, which significantly impacts their optical and spin properties, makes the defect chemically active, rendering a synthetic approach particularly challenging.

In view of these challenges, we investigated the atomic and electronic structure of negatively charged NV⁻ defects in ultra-small nanoparticles, focusing on their chemical stability and photoluminescence resilience. To address the issues with current production techniques, we also explore alternative NX colour centres, which could offer similar spectroscopic properties to NV centres but with more accessible chemical synthesis routes. These alternatives chemically inactive colour centres may present advantages in terms of synthesis, allowing for the controlled production of uniformly small diamond nanoparticles, which is essential to deliver consistent quality and performance. Synthetic approaches using diamondoids as precursors may provide a viable pathway to achieve better control over these parameters.

The exploration of NX centres could lead to advancements in the scalability and cost-effectiveness of ultra-small nanoparticle production, making these materials more.



Keywords: Diamond Color Centers, Photoluminescence, Quantum Computing, Biotechnology

Artificial Kondo lattice in van der Waals monolayer crystals

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The heavy fermion physics is dictated by subtle competing exchange interactions, posing a challenge for their understanding. Conventional heavy fermion systems are found in three-dimensional f-electron materials, which is complicated by the crystal and electronic structures. Artificial heavy fermions not only offer new systems that are simple in structure, but also may add desired functionalities. In this talk, I will present our recent progress in realizing artificial heavy fermions in van der Waals (vdW) monolayer crystals or heterostructures that were grown with molecular beam epitaxy. Utilizing low temperature spectroscopic imaging scanning tunneling microscopy, we observed switching behavior of correlated gap in monolayer 1T-NbSe₂ showing star-of-David (SD) charge density wave (CDW) pattern. Upon decreasing Se flux, a new quasi-1D CDW order emerges as caused by the incorporation of regularly spaced defect lines introduced into the SD motifs. Coherent Kondo screening is established along stripes, forming a long-sought quasi-1D Kondo lattice at the monolayer limit. We also succeeded in constructing a 2D Kondo lattice composed of monolayer VSe₂ grown on NbSe₂, which indicates evident signatures of superconducting heavy fermions via proximity effect from the substrate. Our study realizes artificial Kondo lattices with tailored dimensionality, establishing connection between the heavy fermion physics and 2D materials with desired functionalities.

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Recent Progresses on 2D Charge-Transferonics

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In this talk, we will introduce a model system: synergetic interplay between two layers of 2D interacting electronic system, and the emerging phenomena. Taking the van der Waal hybrid system of graphene/CrOCl for example, due to e-e interactions, the electrons filled (charge transferred from graphene with the help of vertical electrical field) in the surface state (mainly in the Cr-3d orbital in CrOCl, which is about 0.7 nm below graphene) of CrOCl can spontaneously form a long wavelength order, i.e., a Wigner crystal. Such a charge order act as a quantum superlattice, which exerts a moiré-like super potential to the graphene placed on top of it, leading to a series of exotic interaction-driven phenomena [1-4], including unusually robust quantum Hall phase, exciton-enhanced correlated insulator, and interfacial coupling induced p-doping in 2D semiconductors. Our findings suggest that the paradigm of charge transfer can play key roles in the engineering of quantum electronic states, when the e-e interactions are taking effects. According to theory, such a charge-transferred interfacial quantum superlattice and the exotic electronic phases induced therein may be a universal effect, which we define as ‘charge-transferonics’, and enriched physical phenomena are yet to be discovered.

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New electrolytes and electrodes for aqueous Zn batteries

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Aqueous Zn batteries (AZBs) have inspired an overwhelming number of literature studies due to their safety, cost effectiveness, and environmental benignity. Directly employing metallic Zn foil as an anode significantly simplifies battery manufacturing and simultaneously broadens the operating voltage window of aqueous batteries, benefiting from its high overpotential against electrolyte decomposition. Nevertheless, serious issues, such as dendrite growth and side reactions, occurring at the Zn/electrolyte interphase, make the Coulombic efficiency and lifespan of Zn metal electrodes far from satisfactory, which has also been motivating new research interest in interfacial engineering to solve these problems. Owing to the rapid evolution of this new area, it is highly desirable to provide current and timely updates of interfacial strategies and their effectiveness evaluation. From the two sides – the electrode and the electrolyte at the interphase – this report thoroughly summarizes our fundamental understanding of interfacial strategies, including designing mechanisms, creating new methods, and technical challenges. Importantly, this report also analyses the effectiveness evaluation techniques for interfacial strategies, including electrochemical methods, characterization measurements, and computational simulations, providing guidelines for the accurate evaluation and analysis of AZBs in the future.

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Biography

Junnan Hao received his PhD degree in 2020 from the University of Wollongong, Australia. Now he works as a DECRA fellow at the University of Adelaide, Australia. As an early career researcher, he has already demonstrated an exceptional track record, reflected by the publication of 85 refereed papers in peer-reviewed journals, including 3 ESI Hot papers (top 0.1%) and 22 ESI Highly Cited papers (top 1%). These include 35 papers as the first/co-first author and corresponding author, including: *Proc. Natl. Acad. Sci. USA.* (1), *Angew. Chem* (4), *Adv. Mater.* (5), *Nat. Commun.*(1), *Chem. Soc. Rev.* (1), *Energy Environ. Sci.* (2), etc. His research interests are focused on energy storage and conversion, including aqueous Zn-ion batteries, high-voltage Li-ion batteries, dual ion batteries, and flexible energy storage devices. He was also granted by *The Australian Battery Society* as *ABS Energy Renaissance Innovator*, *ARC DECRA*, and *AINSE Early Career Researcher Award* (Australian Synchrotron) etc.

Ferroelectric polarisation as a route to enhancing catalytic and photoelectrochemical performance

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Polarisable multifunctional materials such as ferroelectrics offer new possibilities for extending the performance of photoelectrochemical (PEC) systems beyond what can be achieved with conventional photoelectrodes [1,2]. In this work, we have investigated photoanodes based on the ferroelectric material bismuth ferrite (BFO) for applications in PEC clean fuel generation, e.g. hydrogen generation by water splitting.

In our experimental work, we show that ferroelectric polarisation of BFO can significantly improve the PEC performance. Significantly, we see a larger performance enhancement upon polarisation than in previous studies of ferroelectric photoelectrodes [3,4]. Furthermore, for the first time, we show improvement in performance in both poling directions. By using a combination of analysis methods, we attribute this enhancement to changes in band energies due to the polarisation-induced internal electric field that result in improved charge separation and transport.

Complementing the experimental results, we have used density functional theory (DFT) calculations to show that the surface termination and oxygen content that give the lowest surface energy for BFO depend on the polarisation state. This means that polarisation switching can cause spontaneous release or adsorption of oxygen, so that over a redox reaction cycle, BFO can act as an “oxygen pump”, alternately supplying oxygen for the oxidation half-reaction and adsorbing oxygen to facilitate reduction through switching the polarisation state. In catalytic processes, the material could be dynamically switched between polarisation states to individually optimise the surface chemistry for each step in the reaction process.

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Sustainable materials synthesis through photo(catalysis)

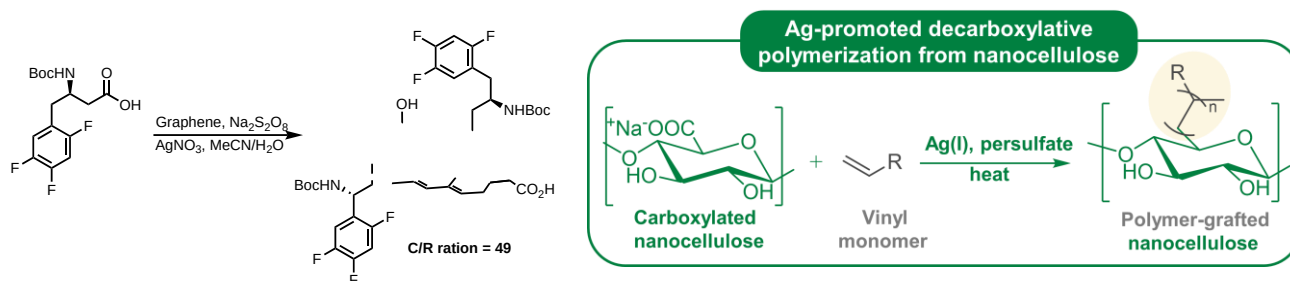
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The synthesis of organic molecules, both big and small, requires efficient processes to access new materials in efficient ways. Catalysis can offer novel methods to deliver new chemical species in economical and sustainable ways.

The synthesis of advanced (bio)polymer materials often requires grafting of small molecules or other polymers. This is typically achieved by functionalising the substrate with a reactive group prior to polymerisation or functionalisation, which can add extra steps and complexity to the process.

In a more ideal approach, grafting would be performed directly from a functional group already present in the starting material, leading to the formation of conjugates via robust C-C bonds in a single functionalisation/polymerisation step.[1-3] One particularly attractive functional group for polymer grafting is the carboxylic acid, which is ubiquitous across biopolymers (polysaccharides, peptides, proteins etc.), synthetic polymers, medicinally relevant small-molecules and natural products. An approach which allows for the controlled grafting of polymers from carboxylic acids would enable the direct synthesis of polymer conjugates of all these materials, leading to a wealth of opportunities for new polymer conjugates and polymer architectures.



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Halide Perovskite Quantum Dot Light Conversion Devices

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Halide perovskite quantum dots are one of the most promising candidates for high-performing and low-cost light conversion electronics due to their unique photophysical properties such as size-dependent bandgaps through quantum confinement effect, unity photoluminescence quantum yield, high light absorption coefficient and high defect tolerance.

In this presentation, Dr Long Hu will showcase the synthesis of high-quality halide perovskite quantum dots (Figure 1a, b), highly ordered self-assembling quantum dot monolayer (Figure 1c), high-performing quantum dot photovoltaics [1, 2] (Figure 1d, e) and luminescence solar concentrator (Figure f).

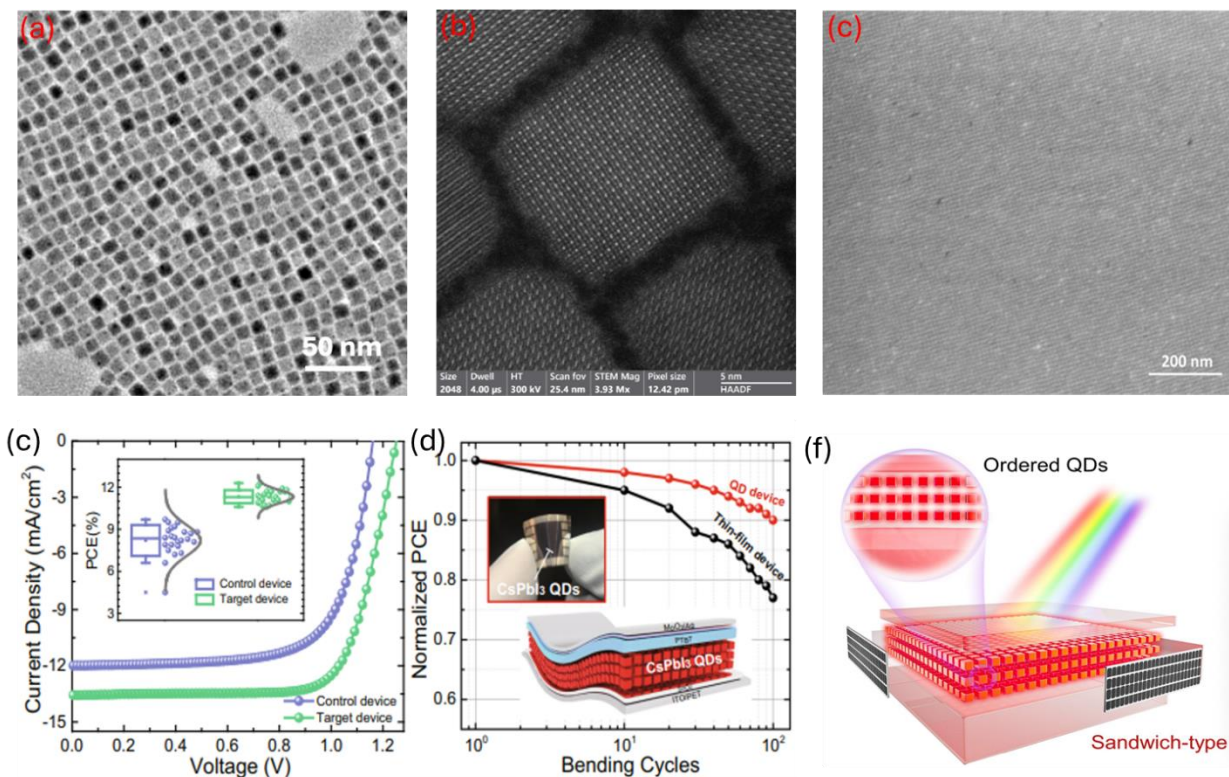


Figure 1. (a) TEM and (b) STEM images of halide perovskite quantum dots, (c) SEM image of highly ordered quantum dot monolayer, (d) J-V curves (e) normalized power conversion efficiency of halide perovskite quantum dot flexible photovoltaics, (f) schematic of quantum dot luminescence solar concentrator

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ABSTRACTS

A Computational Study on Low Dimensional Boron Materials: Structural and Electronic Properties

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Low dimensional boron materials, especially borophene, have attracted broad interests in scientific researches. Here, a novel bilayer borophene has been designed and predicted to be stable by the density functional theory calculations. The normal and high order van Hove singularities emerge in electronic structure of the bilayer borophene, which results in rich of density of states near Fermi level and an ultra-high Fermi velocity of electron. Subsequently, the superconducting behavior of the bilayer borophene has been evaluated theoretically. Moreover, transition metal embedded single layer borophene has been studied, and the key role on electronic structures of supporting metal substrate has been revealed.

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Strong Yet Tough Catalyst-Free Transesterification Vitrimer with Excellent Fire-Retardancy, Durability, and Closed-Loop Recyclability

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Thermosetting resins, one of the most significant polymers, are being widely applied as a resin matrix for fiber-reinforced polymer composites or adhesives in the areas of electric equipment, construction, traffic, and aerospace due to its superior electrical insulation, mechanical strength, and chemical and physical durability [1]. However, most end-of-life thermosetting resins tend to be incinerated or buried, usually seriously impacting the earth's environment and human health.

Introducing dynamic covalent bonds into cross-linked networks has been proven an effective methodology to solve their inability to be recycled. Among them, thermosetting resins based on an associative exchange mechanism are known as vitrimers [2, 3]. The external catalyst, however, can leach out from the vitrimer matrix in the long-term application process, which can cause irreversible damage to the environment and humans [4]. Therefore, it is imperative to develop catalyst-free vitrimers. In addition, the intrinsic flammability and low toughness of thermosetting resins are major barriers inhibiting their high-tech applications [5]. Moreover, due to the presence of dynamic covalent bonds, lots of vitrimers show poor anti-aging, chemical, and creep resistance.

To address the above challenges, a fire-retardant, catalyst-free recyclable transesterification vitrimer (TPN_{1.50}) with superior mechanical properties and durability was prepared by covalently linking an as-synthesized tertiary amine/phosphorus-containing linear oligomer (TPN) to the epoxy/methyl tetrahydrophthalic anhydride network. The bi-phase flame-retardant actions of P-containing groups endow TPN_{1.50} with great fire retardancy. Since the catalytic tertiary amines are fixed in the dynamic covalent network and blocked by rigid phosphorus-based groups, the resultant TPN_{1.50} shows superior chemical/aging/creep resistance, with a topology freeze temperature (T_v) reaching 258 °C, which is higher than those of previous vitrimer counterparts. TPN_{1.50} can maintain structural integrity after being soaked in 1 M HCl or NaOH solution for 2400 hours. In addition, the tensile strength of TPN_{1.50} is as high as 86.5 MPa because of the in-situ strengthening effect of TPN. The outstanding durability and mechanical robustness of TPN_{1.50} make it superior to its existing counterparts. Due to the tertiary amines chemically connecting to the vitrimer network, TPN_{1.50} can be recycled in a closed-loop, and as a polymer matrix to fabricate the advanced carbon fiber reinforced polymer composites, of which both matrix and carbon fibers are chemically recyclable. Hence, this work provides a promising approach for creating high-performance epoxy vitrimers.

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A Zero-Emission Tandem Array for Transforming Waste Biomass into Renewable Hydrogen

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A richness of resources in Australia have seen it be a significant energy exporter to other nations. For instance, in 2021, natural gas exports from Australia were ~\$50 billion AUD. Increasingly though, many countries are seeking to transition away from fossil-fuel derived energy sources to sustainable alternatives, such as renewable hydrogen, however they do not necessarily have the capacity to do so. Given the ongoing shift in the global energy landscape, opportunity exists for Australia to remain a strong energy exporter by contributing to the expansion of renewable (solar) hydrogen into the global energy market. Consequently, there is considerable interest in producing H₂ from electrochemical water splitting in a feasible yet sustainable way for worldwide distribution. While water is known as a renewable and abundant resource, its use as a H₂ source is relatively energy intensive ($>4.5 \text{ kWh mH}_2^{-3}$), is subject to competing uses (e.g., drinking water, agriculture) and is reasonably costly (i.e., the water oxidation reaction is sluggish). These are the key reasons as to why there is a strong urge to develop unique systems to improve the process efficiency, one of which is to use a waste biomass stream in place of water as a feedstock for the electrolyser. A tandem biomass reforming system, comprising a biomass pre-conditioning reactor (BPR) integrated with a flow electrolyser cell (FEC), for extracting H₂ from biomass is put forward for producing zero-emission, renewable H₂ on demand. Biomass oxidation by electrochemical means is selective and scalable, it delivers zero CO₂ emissions and has the additional advantage of producing value-added carboxylic products which can potentially serve as monomers for plastics fabrication.

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Electrochemically induced CO₂ capture with aqueous organic flow chemistryYan Jing^a^a *Department of Materials Science and Engineering, National University of Singapore, Singapore
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Climate change caused by the accumulation of anthropogenic CO₂ emissions motivates the development and deployment of cost-effective, scalable, modular, and energetically efficient techniques to capture CO₂ from point or diffuse sources. Electrochemically-driven CO₂ capture processes utilizing redox-active organics in aqueous flow chemistry and operating at ambient temperature and pressure show promise for nonflammability, continuous-flow engineering, and the possibility of being driven at high current density by inexpensive, clean electricity.^[1-2]

We show that the deprotonated hydroquinone-CO₂ adducts, whose insolubility limits the utility of the quinone-hydroquinone redox couple, become soluble when alkylammonium cations are introduced. Consequently, we introduce alkylammonium groups to anthraquinone via covalent bonds, making the resulting bis[3-(trimethylammonio)propyl]-anthraquinones (BTMAPAQs) soluble.^[3] We report the first aqueous quinone flow electrochemistry induced CO₂ capture/release process, which occurs at ambient temperature and pressure. We show that the electrochemically reduced BTMAPAQs are both Lewis bases and Brønsted bases, thus capturing CO₂ via both a pH-swing and a nucleophilicity-swing mechanism. Among 1,4-, 1,5-, and 1,8-BTMAPAQ isomers, 1,5-BTMAPAQ reaches the theoretical capture capacity of two CO₂ molecules per quinone from 1-bar CO₂-N₂ mixtures for which the CO₂ partial pressure is as low as 0.05 bar, or the applied current density is as high as 100 mA/cm², or the organic concentration is as high as 0.4 M. The energetic cost ranges from 48 to 140 kJ/molCO₂. In a crude simulated flue gas composed of 3% O₂, 10% CO₂, and 87% N₂ with a flow rate of ~12 mL/min, 1,5-BTMAPAQ electrolyte reversibly captured and released 50% of the theoretical capacity during an exposure of over 4 hours. It outperforms its isomeric counterparts 1,4-, and 1,8-BTMAPAQ in capture capacity and O₂ tolerance, demonstrating a substituent position effect on the reactivity of isomers with CO₂ and O₂. The results provide fundamental insight into CO₂ capture with aqueous quinone flow electrochemistry. The oxygen tolerance of reduced quinones may be significantly advanced through molecular engineering by introducing steric and/or electronic effects, intra-molecular interactions, elevating or lowering the oxidation potentials of reduced quinones.

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Engineering Plasmonic Hot-Carrier Transfer at Metal/Semiconductor Interfaces

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Plasmonic catalysis strives to carry out light-driven chemical reactions using plasmonic-metal/semiconductor hybrids. Because plasmonic-metal nanostructures can strongly absorb light, this concept holds the potential to improve solar-to-chemical energy conversion. However, efficiency losses occur in this process because the hot electrons tend to recombine with the holes after they are generated from plasmon decay, without the charges reaching the semiconductor. We investigate bimetallic plasmonic nanoparticles instead of monometallic ones, aiming to boost the mobility of these hot carriers towards semiconductor before their recombination. In our research, we provide evidence that this concept works by choosing the reduction of graphene oxide as a model reaction. Under light exposure, the coupling of GO with Ag-Pt bimetallic nanoparticles resulted in the higher observed conversion, as compared to Ag alone. We will discuss the mechanism by which this improved reduction happens and explain the potential advantages of employing bimetallic nanoparticles.

ABSTRACTS

Thermostable 1T MoS₂ by spontaneous intercalation of Cu single atoms and the enhanced water splitting performance

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We report a simple strategy to fabricate Cu single atoms (SAs) layer-intercalated MoS₂ only by stirring Cu metals with MoS₂ nanosheets solution at room temperature. An ultra-high concentration (Cu: Mo=98 at%) of Cu SAs has been achieved due to the higher chemical bonding energy of Cu-S compared to Cu-Cu, and the intercalated Cu atoms strongly enhance the stability of the thermodynamically unstable 1T-phase MoS₂. Notably, the 1T-metallic phase after Cu intercalation could be maintained even at 800 °C, breaking the record to the best of our knowledge. Besides, the as-prepared MoS₂/SAs exhibit outstanding catalytic performance owing to the improved electrical conductivity and the highly-active unsaturated Cu SAs, and in-situ EXAFS is applied to clarify the catalytic mechanism. This strategy is confirmed as a universal method for producing SAs using other transition or post-transition metals such as Ti, Fe, Ni, and Zn, etc. This work has provided a simple route for synthesizing a high concentration of SAs, which may open a new approach toward the fabrication of low-cost catalysts for a variety of applications including energy devices (*i.e.* battery and supercapacitors, fuel cells), sensors, microwave absorption, and single atom based ferromagnetism etc. Moreover, the high stability of 1T-MoS₂ may make it suitable catalyst applied at high temperature, such as ammonia synthesis and CO₂ conversion. [1]

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Solution-Processed Perovskite Single Crystals and Heterostructures for Opto-/electronics

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Metal halide perovskites have emerged as a promising family of candidates with remarkable physical features combined with facile processing, holding great potential in various photovoltaic and optoelectronic applications. Compared with their polycrystalline counterparts, single-crystal perovskites, due to their absence of grain boundaries and high crystallinity, feature reduced trap density, enhanced absorption properties, improved charge carrier dynamics, and outstanding stabilities, demonstrating significant potential in advanced optoelectronic devices.^[1]

Recently, we reported that solution-processed perovskite single crystals and the related heterostructures (including epitaxial, lateral, and vertical ones) can be used to develop the high-performance and cost-effective electronic and optoelectronic applications, like transistors and photodiodes, which show great promise for the real-world applications. In this talk, I introduce our recent works on optoelectronic and electronic devices based on halide perovskite single crystals and the related heterostructures. I will present how we applied spatially confined inverse temperature crystallization technology to grow high-quality micrometer-thin epitaxial perovskite thin single crystals, which were used as the active layer in transistors, achieving high carrier mobility and on-off ratio, as well excellent stability.^[2] Following this, I will introduce how high-quality 2D-3D mixed-dimensional perovskite single-crystalline lateral heterostructures can be realized through a one-pot solution synthesis approach. Benefiting from the built-in field that effectively suppresses the dark current and separates the photogenerated carriers, the proof-of-concept photodetectors exhibit a low dark current of less than 0.01 nA and a champion detectivity exceeding 10^{13} Jones.^[3]

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Developing New Regenerative Therapies for Bone and Joint Diseases

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Musculoskeletal conditions including bone and joint diseases are leading contributors to the chronic disease burden, affecting 1 in 3 people worldwide. In addition to causing significant disability and decline in quality of life, they also greatly increase the risk of death from other concurrent diseases such as cardiovascular disease. These conditions have no cure, and their long-term management imposes an enormous burden on global healthcare systems.

My research program based on tissue engineering and regenerative medicine has the broad aim of fulfilling unmet clinical needs in treating chronic bone and joint conditions. There is a huge clinical problem with repairing large areas of bone loss arising from traumatic injury or surgical procedures, due to the drawbacks experienced with currently available bone grafts [1]. One aspect of my research involved the development of new synthetic grafts made from bioceramics for bone repair and evaluating them in large animal models, in challenging scenarios replicating clinical cases. This work served as a cornerstone in developing world-first implants that help regrow natural bone, and in bringing Australian inventions to the global orthopaedic market.

My current research focuses on developing regenerative therapies for joint diseases, using osteoarthritis as a model disease. All clinical treatments for osteoarthritis only relieve pain rather than stop disease progression. Stem cell therapies have recently emerged, among which mesenchymal stem cells (MSCs) have been the most commonly tested due to their natural anti-inflammatory and restorative functions [2]. However, the efficacy of MSC therapy for osteoarthritis treatment is limited by some key factors, which our team has sought to address by (1) using microcarrier systems to improve the efficiency of cell delivery and cell viability after injection, (2) optimising 3D culture methods to enhance MSC paracrine activity.

Interestingly, our recent work also demonstrated that live MSCs may adopt the diseased characteristics of the osteoarthritic joint after injection, hence reducing their long-term therapeutic benefits [3]. This prompted us to look into the MSC secretome, and generate cell-derived bio-therapeutics as a new treatment option for osteoarthritis. We hope that our combined therapeutic discovery strategy can in the future be adapted for other types of chronic diseases.

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Biomaterial nanocomposites in agriculture

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A topical spray of agrochemical formulations is a convenient and popular approach to protecting the plant and enhancing the crop yield. However, agrochemical utilisation efficiency remains relatively low due to the runoff of sprayed drops from leaves. After the topical spray leaves the nozzle, only about 10-40% of sprayed agrochemicals are deposited on leaves due to the superhydrophobic nature of most leaf surfaces. The poor adhesion and retention of sprays on foliage results in inefficient agrochemical delivery. To address this issue, we have developed biomaterial nanocomposites as platforms for the precision delivery and release of various agrochemicals to improve their performance and reduce their environmental impact. Using these biomaterial nanocomposites, we have demonstrated a significant enhancement of herbicide and RNAi attachment on the leaf surface and their resistance against washing/raining upon cellulose involvement, indicating a general approach to enhancing the efficiency of topical sprays using these biomaterial nanocomposite formulations.

The *panoscopic* approach to low thermal conductivity

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Low thermal conductivity is favorable for many applications, including thermoelectrics, photovoltaics, and radiative cooling.[1] The key to achieving low-thermal-conductivity functional materials lies in suppressing the propagation of lattice vibrations (phonons) in both intrinsic and extrinsic schemes. Intrinsically, this contains the modification of normal and Umklapp processes plus intensifying diffusive and localized modes, mainly through engineering Einstein rattlers, lone pairs, chemical bonds, and lattice harmonicity. Extrinsically, this is related to introducing all-scale lattice defects to scatter phonons in hierarchical frequencies, such as point defects, stacking faults, grain boundaries, and nanoprecipitates. It is also noteworthy that the nanoprecipitates with unique physical properties may induce additional electron–phonon or magnon–phonon interactions toward an even lower thermal conductivity. The effort to integrate all these mechanisms simultaneously and additively, if not synergistically, into a single material is termed the *panoscopic* approach.[2] This presentation shows the theoretical and experimental investigations conducted by our research group recently in achieving low-thermal-conductivity thermoelectric materials,[3–5] which are transferrable to other functional materials.

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Microscopic carrier loss mechanisms in kesterite $\text{Cu}_2\text{ZnSn}(\text{S,Se})_4$ thin film solar cells

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Emerging inorganic thin-film solar cells are attracting considerable attention for their huge potential of diverse applications scenarios in the modern and future society. While the power conversion efficiencies of these emerging thin-film solar cells are limited for some reasons, mostly associated with microscopic carrier loss mechanisms. In this talk, I will discuss our recent works on carrier loss mechanisms in kesterite solar cells: the roles of interfacial recombination, grain boundary recombination, and bulk recombination respectively and how to identify the dominant microscopic carrier loss mechanisms in polycrystalline thin-film solar cells^[1]. Using $\text{Cu}_2\text{ZnSnSe}_4$ (CZTSe) as an example, we discuss how multiple micro- and macro-scale characterizations are applied to investigate the most important carrier transport and carrier recombination mechanisms, and how these characterizations are integrated with the 3D device simulations^[2].

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Management of local ionic transport for stable CO₂ electrolysis

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

Exploration of C–N Coupling for Electrocatalytic Urea Synthesis

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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 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.

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Thermoelectric technology for low-grade waste heat recovery

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Thermoelectric technology, with the capacity of direct and reversible energy conversion between heat and electricity, has attracted extensive research interest. The performance of thermoelectric technology fundamentally dominated by the material dimensionless figure of merit, zT . And higher zT values of composing thermoelectric materials correspond to high energy conversion efficiency. Obtaining high zT values of thermoelectric materials is typically limited by the coupling relationship between sub-parameters of thermoelectric materials, including electrical conductivity, Seebeck coefficient, and thermal conductivity. Here, based on our state-of-art studies focusing on Bi_2Te_3 - and $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ -based materials, we proposed the strategies of obtaining high-performance thermoelectric technologies by decoupling these relationships from material viewpoint, where the synergistic carrier concentration optimization under decoupled sub-parameters can contribute to high zT values in both n-type Bi_2Te_3 -based and p-type $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ -based materials. For practical application, high efficiency and power density are of equal significance, where novel thin-film device design can effectively approach this target, which has been realized by the combination of magnetron sputtering and flip-chip bonding techniques. Meanwhile, effective application of thermoelectric technology, such as personal thermal management or chip cooling, requires comprehensive system optimization, which has also been demonstrated in our preliminary studies.

Unveil the Triple Roles of Water Molecule on Power Generation of MXene Derived TiO₂ based Moisture Electric Generator

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Abstract: Evaporation-driven electricity generators have been proposed to generate electricity by water interacting with nanostructured materials. However, several proposed mechanisms, such as intrinsic gradient of polar functional groups principle and electrokinetic effect perspective, are in wide discrepancy. Here, through the combination of theoretical calculations involving time dimension on material's moisturizing process and experimental analyses, it is revealed the working principle through the water molecule triple roles in driving moisture electric generators (MEGs): 1) intrinsic H₂O absorption on the material surface and splitting into hydroxy group and proton due to the polarizability of the material surface determined by the static electric potential of the materials. This process induces the electrochemical potential difference of the materials via the work function changes; 2) freely diffused protons derived from the H₂O splitting work as the ions charge carriers; 3) via the hydrogen bond of the water molecules to drive charge carriers diffuse between opposite electrodes, maintaining the internal circuit current flow. It is successfully unveiled that anatase TiO₂ based materials for output voltage changes correlated to the domains' work function's difference, tuning by the surface adsorption species (H, Cl, OH) and anisotropic exposed crystal facets of the material. This work unveils MEG's general working principle.

Diketopyrrolopyrrole Polymers: N-dominant Feature for Molecular Doping, Flexibility and Stretchability Studies

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Diketopyrrolopyrrole (DPP) is a promising block to design organic semiconductors for various (opto)electronic devices [1]. However, how to develop n-dominant DPP materials, followed with n-dominant doping studies and n-type flexible and stretchable devices are extremely challenging. In this presentation, in terms of DPP materials, I will talk about the effects of flanking groups of DPP on promoting n-type feature [2-4], influences of dopants on both the holes and electrons transport [4-7], hybrid effects of DPP materials on the performance of black phosphorus [8], and feasibility for high-performance n-type flexible and stretchable devices [9].

Specifically, tuning the electron affinity of flanking groups of DPP is a powerful strategy to convert the charge carrier polarity from p- to n-type feature; the synergistic use of pyridine and selenophene decreased both the HOMO and LUMO levels, which suppress holes injection and facilitate electrons injection, respectively, for more n-type feature; the hybrid of black phosphorus and a low band-gap DPP polymer enhanced the holes and electrons mobility, broadened photodetection ranges and responsibilities in ambient atmosphere; through careful doping control, a precise tuning of charge carrier polarity from a p-dominant to a balanced to a n-dominant and to a nearly unipolar n-type feature was achieved, and a pioneered result to simultaneously enhance the holes and electrons mobility in a single polymer with any of three selected dopants was first observed, which is often a conflict according to commonly recognized doping mechanism of electron transfer. Finally, aiming for skin-like electronics, we developed a simple yet efficient strategy to demonstrate a best n-type stretchable mobility.

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Multiscale structural parameters affecting properties of polar functional materials

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Polar functional materials, particularly ferroelectrics (FEs), are essential in modern electrical and electronic devices such as capacitors, sensors, and FeRAM. Recently, antiferroelectric (AFE) materials, characterised by their antiparallel-aligned polar order, have raised research interest due to their potential in energy conversion and storage applications.^[1] To innovate and advance novel polar functional materials, understanding the structure-function relationship is essential. However, in most cases, a single descriptor like the average structure is inadequate for interpreting observed properties. Therefore, it becomes pressing to explore the structural parameters at various length scales. This presentation will highlight the significance of multiscale structural parameters by focusing on two niobate examples^[2]. Although their average structures are centrosymmetric, which typically prohibits polar functionalities, they exhibit unusual properties related to the inherent polarisation. By using total scattering techniques combined with reverse Monte Carlo modelling, we have successfully identified the nano polar clusters formed by local atomic displacements in these niobate materials, and this critical structural information is not apparent from diffraction data alone. Most importantly, nano polar clusters effectively explain the unusual polar features. Therefore, this study provides a new strategy to expand the candidate pools of polar functional materials through rational chemical and local structure design.

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Next-generation Energy Devices for Low-Power Internet-of-Things Devices

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The advent of the Internet-of-Things (IoT) era has witnessed an exponential growth of wearable and flexible electronic devices.[1] These IoT devices generally feature good flexibility, wireless operation and low power requirements, which in turn poses high demand on new form factors of portable energy devices that can serve as cost-effective integrated power sources.[2] Flexible zinc ion batteries are ideal energy storage candidates due to their low-cost, high safety, high volumetric energy density and ambient printability, while indoor photovoltaic offers a promising solution as a sustainable source.[3-5] Some research work has been conducted to address these two topics. We developed a rechargeable electrolyte that can be printable in ambient conditions for flexible zinc-ion batteries, which is promising for flexible power sources for IoT devices. In addition, efficient indoor photovoltaics based on halide perovskite have been achieved through a solvent engineering strategy, which can effectively suppress the defects in the perovskite layer and significantly enhance the device performance under low-light conditions.[4] Interestingly, the solvent engineering approach can also tune the transparency of halide perovskite films, leading to efficient semitransparent indoor solar cells.[6] We hope the research work can shed light on the next generation of energy devices for powering wearable and flexible IoT electronic devices.

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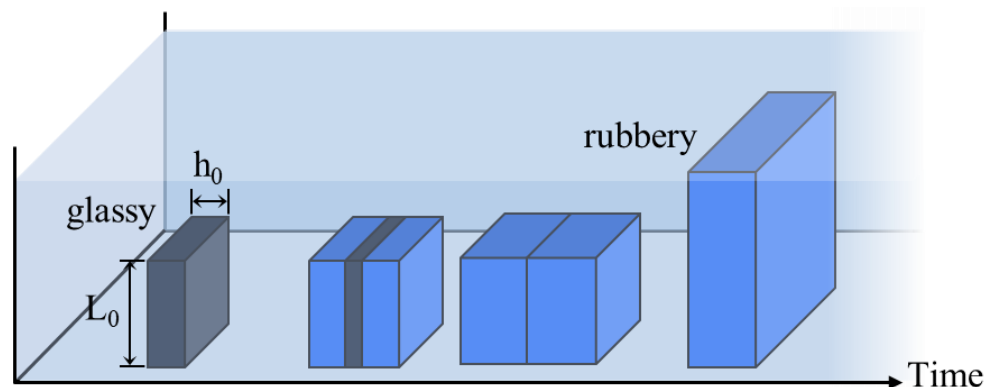
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Case II Diffusion and Anomalous Swelling of Glassy Polymers

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A sheet of glassy polymers placed in solvent shows a swelling behavior quite different from that of soft polymers (rubbers and gels). In the classical work of Thomas and Windle, they reported the following characteristics in the swelling of PMMA in methanol. (1) Non-Fickian diffusion (called case II diffusion): the thickness of the sample increases in time in proportion to the time t instead of following the Fickian diffusion law. (2) Anomalous swelling: The thickness first increases, while the area remains constant. After some time, thickness starts to decrease in time, while the area starts to increase, towards the equilibrium value. Such behaviors have been observed for other polymers, e.g., PVC with acetone, PS with alkane, and samples with other geometry. Moreover, case II diffusion appears in other systems, like the permeation of ions into conjugated polymers and so on. We propose a three-dimensional theory for the swelling of glassy polymers. We show that this simple model explains all anomalies observed in the swelling of glassy polymers. The theory also predicts how the permeation speed of solvent and the characteristic times depend on material parameters and experimental conditions. It provides effective ways to control the swelling of glassy polymers.



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Coupled NO_x Production and Electrochemical NO_x Conversion Processes for Renewable Ammonia Synthesis from Air

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Decarbonization of economy is dependent on the uptake of renewable electrification as well as Power to X pathways,¹ especially for regional energy application and agricultural production. Amongst these pathways, decentralized Power-to-Ammonia module is projected to play a big role in attaining net-zero emissions as it will enable the reach of renewable electrons to substitute diesel consumption for mobility in mining and farming applications, as well as providing zero-carbon fertilizer for agriculture. This potential of renewable ammonia is increasingly recognized by industry and government, with a number of renewable hydrogen project developers substituting fossil-fuel sourced hydrogen with renewable hydrogen that is then used in energy-intensive Haber-Bosch (HB) process to generate renewable ammonia.² While such an approach allows operation of existing HB plants with modification to avoid assets being stranded, this pathway requires high temperature and pressure, presenting challenges for intermittent renewable integration to run the process and at the same time being capital-intensive, thereby limiting the scope of decentralized on-demand production.^{3, 4}

To this end, we report a simple, scalable, and continuous hybrid pathway coupling air oxidation technique with electrolyzer to convert air and renewable electricity to ammonia, while the side produced O₃ can also serve as irrigation water purifying agent when using the coupling system for fertilizer supply in agriculture. Specifically, the plasma reactor converts air into gaseous O₃ and NO_x, which can be directly introduced into a flow electrolyzer equipped with a Cu-based multi-phase-electrode (MPE) with gas-diffusion-layer to allow the delivery of the gaseous NO_x to catalyst sites for further conversion into NH₄⁺. The unreacted NO_x can be directed into water for producing nitrate solution, which could be pumped back into our custom-designed electrolyzer as catholyte where they can be converted to NH₄⁺ on the catalysts from liquid side of Cu-based MPE. Meanwhile, the generated ozone with tunable production rate from 0.01 to 1.2 μmol min⁻¹ could also be used for water treatment on demand. As such, the as-designed plasma reactor-electrolyzer system is capable for converting air (N₂ and O₂) into reactive NO_x species (both in the forms of gaseous NO_x and ionic NO_x⁻), which promoted their further conversion into NH₄⁺. The efficient NH₄⁺ production (1.3 mmol h⁻¹ cm⁻²) and low energy consumption (<100 kWh kg_{NH₄⁺}⁻¹) of the coupling system make it feasible to be directly powered by a solar panel for achieving the renewable Power-to-Ammonia.

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ABSTRACTS

Coherent Ag-rich Nanoprecipitates/ β -Ag₂Se Flexible Film with Unprecedented Thermoelectric Performance by Liquid-like Sintering

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β -Ag₂Se holds great promise for wearable thermoelectric generators due to its good mechanical properties and biocompatibility, however, optimizing its power factor (PF) through alterations in the Ag/Se stoichiometric ratio or incorporating secondary phases has reached the limitation. This work adopts a liquid-like sintering strategy, namely employing the migration and precipitation of silver ions from metallic silver to the silver selenide during the spark plasma sintering process to construct significantly sized and coherent Ag-rich nanoprecipitates within flexible Ag/ β -Ag₂Se composite films, thereby achieving an unprecedented power factor exceeding $4000 \mu\text{W m}^{-1} \text{K}^{-2}$ at 303 K. The Ag-rich nanoprecipitates play a crucial role in elevating the carrier concentration, enhancing the effective mass of the density of states, and mitigating carrier scattering caused by phase interfaces and acoustic phonons. The film with an optimal length exhibited a large output power density up to $12.09 \mu\text{Wcm}^{-2}\text{K}^{-2}$ under a temperature difference of 17.4 K. This study strongly suggests that the creation of Ag-rich nanoprecipitates is an effective avenue for improving the electrical performance of β -Ag₂Se-based thermoelectric materials.

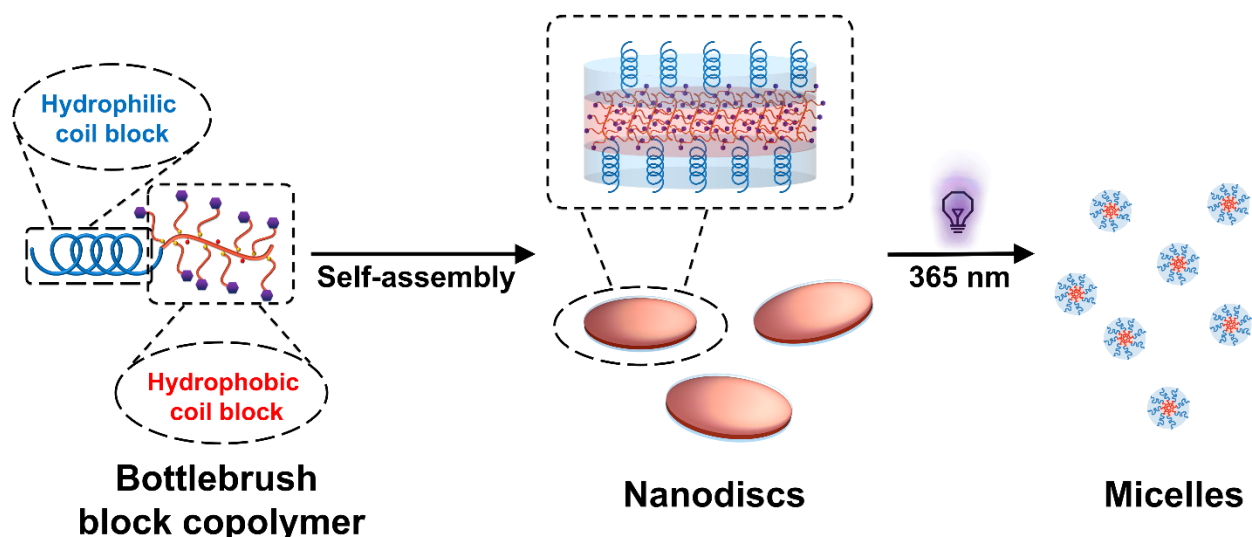
Self-Assembly of Amorphous and Functional Polymer Nanodiscs in Water

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Polymer nanodiscs are challenging to make.[1] This is because self-assembly processes typically yield micelle shapes of minimised energy, like spheres or vesicles. Flattening such assemblies is more intricate, as block ratios and solvent—polymer interactions alone cannot compensate for the energy costs to flatten a curved surface or interface. Taking on this challenge, we designed an amphiphilic, tadpole-like copolymer featuring a hydrophilic linear block and a hydrophobic bottlebrush block.[2] The linear segment assumes a coil-like conformation, while the bottlebrush segment adopts a stiffened, rod-like structure. Using this rod-coil architecture facilitated planar packing of brush segments and yielded nanoscale polymer discs via spontaneous self-assembly. A characteristic feature of this methodology is the possibility to select the chemical composition of the brush segment without compromising the disc formation. This allows the introduction of functionality into these amorphous core-shell nanodiscs, enabling triggered disassembly and/or drug release, depolymerisation, or shape-transformation. My talk will introduce our general approach.



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Mixed-mode interpenetrating polymer networks from polymerizable eutectics

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Deep eutectic solvents (DESs) have been explored over the past 20 years as an alternative to many traditional solvents. There are several classes of DESs and the most commonly utilized is a combination of hydrogen-bond donor (HBD) and hydrogen bond acceptor (HBA) species, forming a stable mixture with a lower melting point compared with the individual components.^[1] In the context of materials chemistry, polymers can be prepared in a DES or from a polymerizable eutectic mixture, where one or more of the components is a monomer. Previous studies have shown enhanced polymerization kinetics and material properties when preparing polymers from or in a eutectic mixture as compared with a traditional solvent.^[2-5] Many commercially available monomers can also act as HBDs or HBAs in a eutectic mixture, allowing for the design of a wide variety of simple and cheap polymerizable eutectics.

N-isopropylacrylamide (NIPAM) and ϵ -caprolactone (CL) can be polymerized through different modes, and they readily form a eutectic mixture with a melting point of -15 °C at a 1:1 molar ratio. Previous work on this polymerizable eutectic explored the formation of PNIPAM-PCL block copolymers through simultaneous photoinduced-electron/energy transfer-reversible addition-fragmentation chain-transfer (PET-RAFT) of NIPAM and ring opening polymerization (ROP) of CL. This was achieved using a bifunctional ROP initiator/PET-RAFT chain transfer agent and the polymerizations were shown to be semi-orthogonal.^[3]

The current work investigates the one-pot, mixed-mode polymerization of NIPAM-CL polymerizable eutectics using a range of radical and ROP catalysts to form interpenetrating polymer networks. The orthogonality of these polymerizations is explored along with polymerization kinetics, and material properties of gel networks prepared from this method.

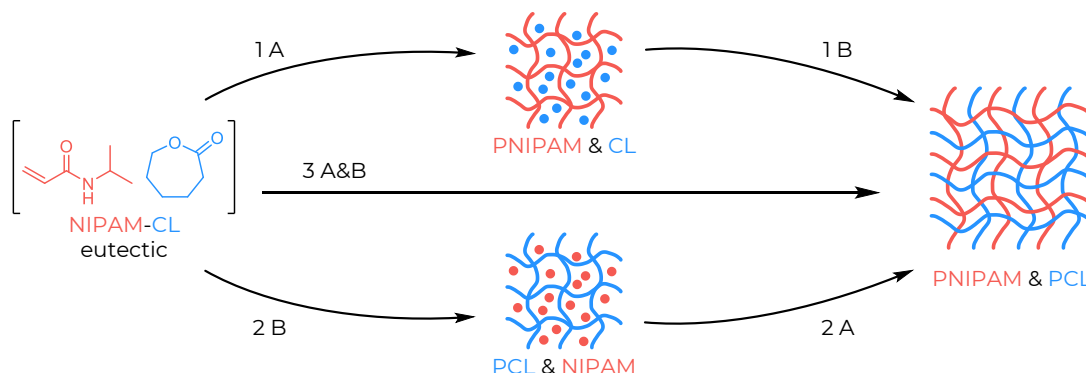


Figure 1. Scheme showing simultaneous and sequential preparation of PNIPAM and PCL networks from a eutectic mixture. Reactions labelled ‘A’ use photoinitiator and irradiation. Reactions labelled ‘B’ use an ROP catalyst & initiator.

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Engineering 2D van der Waals materials for polariton nanophotonics

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Manipulating photons at the nanoscale and developing low-loss on-chip photonic and optoelectronic devices are the focus of research in the field of nanophotonics. The key issue is how to achieve high confinement and propagation control of light in the 2D plane. Polaritons, hybrid light-matter waves, enable nanoscale control of light. Particularly large polariton field confinement and low losses have been found in graphene and 2D van der Waals materials.

In this talk, I will present our recent progress in manipulating in-plane hyperbolic phonon polaritons from the perspective of material engineering [1]. Firstly, by fabricating twisted α -MoO₃ bilayers [2] and van der Waals heterostructures [3], we experimentally observed photonic magic angles and tunable topological transitions of phonon polaritons. At the transitions, the photonic dispersion flattens, exhibiting low-loss tunable polariton canalization and diffractionless propagation. Secondly, via structural engineering, we demonstrate unidirectional excitation and diffraction of hyperbolic polaritons [4] and low-symmetry Bloch modes in hyperbolic polaritonic crystals [5]. Lastly, we show monolithically structured van der Waals hyperbolic crystals for planar refraction and focusing of volume-confined phonon polaritons [6].

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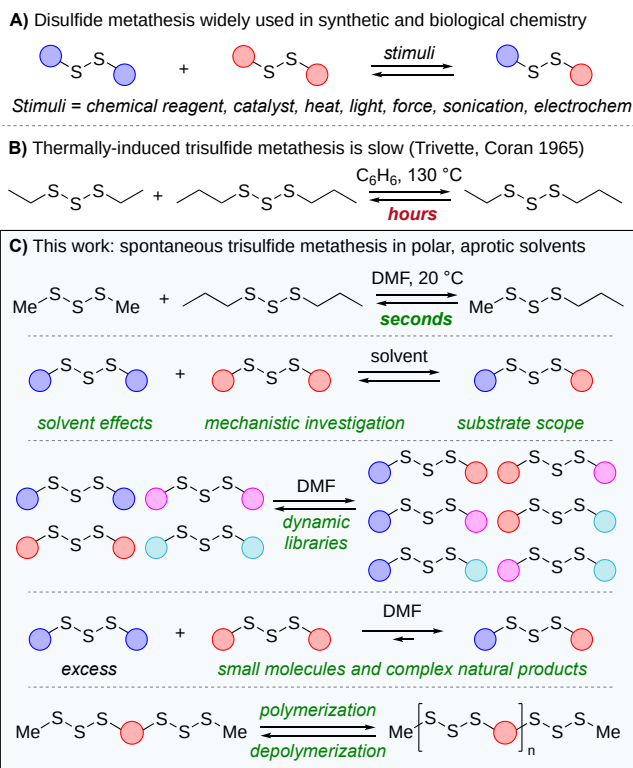
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Spontaneous Trisulfide Metathesis in Polar Aprotic Solvents

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Sulfur-sulfur bonds are ubiquitous across broad classes of natural products, peptides and proteins, drug molecules, and synthetic polymers and materials. The ability to make and break these bonds in a controlled manner is critical for their many scientific and technological applications. In this study, we report the discovery of a new and unusual S-S metathesis reaction of linear organic trisulfides. When exposed to certain polar aprotic solvents, trisulfides were found to undergo spontaneous metathesis, with equilibrium established in seconds in some cases. No exogenous reagents, heat, light, or other stimuli were required to provoke this reaction. Understanding the scope and mechanism of this reaction enabled diverse applications of this chemistry in dynamic combinatorial library synthesis, covalent modification of complex natural products, and S-S metathesis polymerization and depolymerization as a platform for chemically recyclable plastics (Figure 1).¹ The discovery of this new and efficient reaction bodes well for application to the many emerging applications of sulfur-rich polymers.²⁻⁴



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Understanding the roles of the acceptors in organic solar cells with a ternary blend

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Organic solar cells (OSCs) have attracted significant attention from both the academic and industrial sectors due to their attractive features of being lightweight and structurally conformable, along with their viability for high-volume low-embedded energy manufacturing. Improvements in power conversion efficiency (PCE) can be achieved by adding a third component into a host binary bulk heterojunction (BHJ) OSC, containing a donor and an acceptor, to form a ternary device.^[1] The third component in a ternary organic solar cell is generally selected to maximise the light absorption with respect to the solar spectrum but in doing so it must not introduce trap states that might impede charge extraction from the active layer.

We have synthesised a fused ring non-fullerene acceptor (o-IDT-BT-DCV) for use in ternary organic solar cells. The optimised binary device used o-IDT-BT-DCV as the acceptor and PM6 as the donor had a maximum power conversion efficiency (PCE) of 10.8%. o-IDT-BT-DCV was then blended into a host PM6:Y6 mixture with composition ratios ranging from 10% to 40% of the total acceptor weight to form a ternary blend. To further enhance the PV performance of the PM6:Y6:o-IDT-BT-DCV ternary blend we explored the use of the solid additive 1,4-diiodotetrafluorobenzene (1,4-DITFB), which has been reported to change the crystalline/domain size and molecular packing of PM6:Y6 binary devices, leading to a dramatic improvement in device efficiency.^[2] The incorporation of o-IDT-BT-DCV into a donor:acceptor PM6:Y6 blend and optimisation of the film structure delivered a ternary organic solar cell with a maximum PCE of 16.2%.

The exciton dissociation and charge generation processes were investigated using femtosecond transient absorption spectroscopy (fs-TAS). The results showed that o-IDT-BT-DCV in the ternary blend was no longer behaving as an acceptor, as it was in the binary film with PM6. Instead, it contributed to charge carrier generation through a sub-picosecond energy transfer process to Y6, which then generated charge through a photoinduced hole transfer mechanism with PM6 and/or spontaneous exciton dissociation within the Y6 phase. Encapsulated devices composed of the ternary blends were found to be more stable after the initial burn-in. Under 1-sun illumination and maximum power point tracking the ternary device lost only ~30% of its efficiency over 1200 h whereas the PCE of the PM6:Y6 binary blend decreased by around 60% over the same timeframe. In summary, the incorporation of a second NFA acceptor into a PM6:Y6 binary blend was found to lead to alternate charge generation pathways that improved PCE with the added benefit of enhancing device stability.

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Functional Polymer Electrolyte Design for Efficient Zn Batteries

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Merited by their intrinsic advantages of safety and low-cost, rechargeable Zn batteries are emerging as a promising energy storage technology complementary to Li batteries. [1-2] The nature of the electrolytes greatly demarcates the electrochemical performance of Zn batteries. In recent years, polymer electrolytes have been widely investigated in various types of Zn batteries due to their unique physicochemical properties. In this talk, I will present our recent advances in the design of functional polymer electrolytes for efficient Zn batteries, including those availing the desolvation of Zn^{2+} charge carriers, flexible molten hydrate salt electrolytes, solid-state single Zn^{2+} conductors, gel electrolytes with intrinsic wide temperature-adaptability, and the intrinsic catalytic properties of typical polymer electrolytes. [3-6]

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Liquid Metal Integrated Hybrid Materials as 4D Printing Soft Robots

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Soft robotics is a rapidly expanding frontier in research, with diverse applications ranging from general robotics and microrobotics to drug delivery, surgery, tissue engineering, optical devices, and foldable electronics. However, advancing soft robots to perform complex tasks requires significant innovations from the materials science community.[1] This talk will highlight our recent work in liquid metal-integrated hybrid materials,[2] including the surface engineering of liquid metal,[3, 4] the fabrication of 4D-printed soft robots,[5] and our latest study on hybrid soft robotics. Notably, we have developed a single-step process to directly fabricate soft robots with precisely controlled mechanical properties.[6]

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Exfoliation and Functionalization of Layered Double Hydroxides (LDHs) for Catalytic and Energy Applications

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Two-dimensional (2D) layered double hydroxides (LDHs) with adjustable composition and structure have been promising candidates for various domains including catalysis, water treatment, and energy storage. To unlock their full potential, various exfoliation methods for producing 2D LDHs with different size, morphology and surface functionalities have been explored.

We reported the preparation of a series of LDH nanosheets (CoAl-LDH, MgAl-LDH, ZnAl-LDH, and NiFe-LDH) by a solid-phase exfoliation technique. Surface functional groups and defects are introduced into the exfoliated LDHs, which enhance the long-term aqueous dispersion stability of LDH nanosheets. The induced defects introduce more active sites which enhance their electrocatalytic performance. The exfoliated NiFe-LDH nanosheets show a superior OER activity with an ultralow overpotential of 258 mV at 10 mA cm⁻².

Furthermore, LDH nanosheets (MgAl-LDH) with varying surface charge has been studied. The tunable surface charge density is enabled by the controlling the stoichiometric ratio of the metal ions. Ion selective membranes (ISMs) based on these LDH nanosheets preferentially facilitate anion transport with high selectivity. Osmotic energy harvesting device based on these membranes reached a power density of 2.31 W m⁻² under simulated river/sea water. Prototype reverse electrodialysis (RED) energy harvesting device, comprising a pair of LDH membrane and commercial cation selective membrane, was able to simultaneously harvest energy from both cations and anions achieving a power density of 6.38 W m⁻² in simulated river/sea water, demonstrating its potential as building blocks for future energy harvesting systems.

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Atomic-Level Regulation on Photocatalyst for Energy-Related Reaction

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

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Advanced nanostructured metasurfaces

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Ultrathin metasurfaces, comprised of a surface array of engineered nanostructures, have transformed the landscape of photonic design, driving significant technological advancements in areas such as optical imaging, displays, AR/VR, LiDAR, and molecular sensing. Beyond wavefront-shaping metasurfaces that precisely control local light scattering, spatially homogeneous metasurfaces can resonantly couple light into nonlocal optical modes with sharp resonances. In this presentation, I will highlight our recent work on the design and fabrication of tunable bound states in the continuum (BIC) metasurfaces using an ultrathin and ultralow-loss Sb₂Se₃ phase-change materials. Our BIC metasurfaces, only 25 nm thick, achieve broad resonance tuning in the near-infrared region with high-quality (high-Q) factors up to 130, without the need for foreign materials. Experimentally, we employ these BIC metasurfaces to enhance photoluminescence in rare earth-doped upconversion nanoparticles, significantly reducing the excitation power threshold for multiphoton photoluminescence and enabling emission polarization manipulation. Additionally, I will introduce the use of BIC metasurfaces for highly sensitive molecular sensing [1], leveraging metasurface-tailored light-matter coupling between light and molecular analytes.

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Topological Structures in Multiferroic Oxide Thin Films and Superlattices for Future Low Energy Computation

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The information and communication technology sector presently consumes around 7% of the world's electrical power, and this is projected to account for 20% by 2030. Sustainable growth in information technology requires the development of new approaches that consume less energy. Topological defects (or “solitons”) in *multiferroics* – materials that exhibit ferroelectricity and magnetism – are promising candidates for future computation by virtue of their ultrafine size, sensitivity to various external stimuli including electric and magnetic fields, and ultrafast time-dependent response.

In ferroelectrics – materials that possess a spontaneous electric polarization that can be switched with low energy electric field – the competition among various degrees of freedom leads to rich phase diagrams and the possibility to create topologically protected polarization textures including solitons. In thin films, the ability to tune mechanical and electrical boundary conditions by epitaxial strain, substrate orientation, and superlattice design, offers a versatile route to designing such structures [1].

In this presentation, I will summarise our efforts to craft new topological polar textures in the popular multiferroic BiFeO₃ (BFO). This material combines ferroelectricity with antiferromagnetism (both available at room temperature), providing a wider palette of functional properties for computation (e.g., responding to both electric and magnetic fields). By combining BFO with SrTiO₃ in carefully designed superlattices, we engineer the formation of ferroelectric solitons [2]. High-resolution piezoresponse force microscopy and atomic resolution transmission electron microscopy uncover a zoo of topologies, including centre-convergent/divergent topological defects as small as 3 nm. Phase field simulations and effective Hamiltonian computations reveal that some of these structures can be classed as “bimerons” with a topological charge of ± 1 , while others can give non-integer topological charges, a first observation in a BiFeO₃-based system.

As these topological defects can possess drastically different electronic properties (band structure, spin texture, etc.) than the bulk material that surrounds them, we plan to incorporate multiferroic solitons into micro and nanoscale tunnelling devices, with a view to control the quantum states within the device using applied voltages, magnetic fields, light, etc. Our work is an important stepping stone for the next generation of beyond-silicon computation based on multiferroic solitons, providing new opportunities for these material systems.

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Electronic Structure Studies on Altermagnetic Candidates: CrSb and RuO₂

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Altermagnetism(AM) has been proposed as a third fundamental magnetic phase beyond traditional ferromagnetism and antiferromagnetism in crystals with collinear magnetic order. Electronic structure probing techniques like angle-resolved photoemission spectroscopy (ARPES) and spin-resolved ARPES (SARPES) can detect momentum-dependent band splitting and spin polarization induced by AM, considered the gold standard for identifying AM order in compounds.[1-3]

Employing high-resolved Micro-ARPES beamline (BL03U) at SSRF, we performed a focused investigation of these materials, especially CrSb, and mapped its three-dimensional electronic structure. Due to accurate Brillouin zone positioning, our results on the (001) and (100) surfaces of CrSb consistently confirmed its AM characteristics. Notably, the band splitting near the Fermi level reached up to 1 eV, the highest value recorded among all confirmed AM materials to date. [4]

For the other workhorse material of RuO₂, we employ (S)ARPES to investigate the band structures and spin polarization of both thin-film and single-crystal. Contrary to expectations of AM, our analysis indicates that RuO₂'s electronic structure aligns with those predicted under nonmagnetic conditions, exhibiting no evidence of the hypothesized spin splitting. Additionally, we observe significant in-plane spin polarization of the low-lying bulk bands, which contrasts with the d-wave spin texture due to time-reversal symmetry breaking in AM. [5]

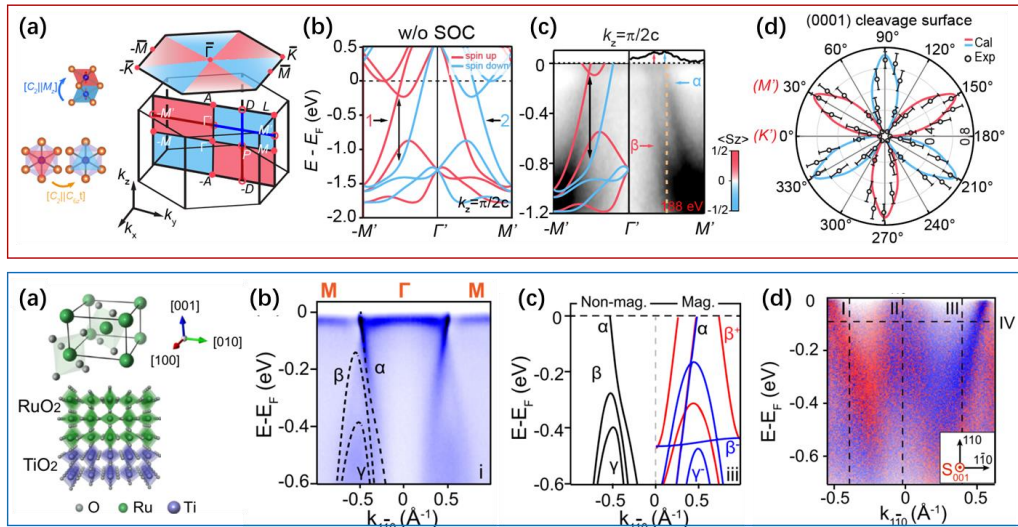


Figure 1 upper panel: Spin sublattices symmetry and spin splitting bands in CrSb crystals, lower panel: band dispersion along Γ -M and its corresponding spin polarization in RuO₂.

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The next generation ultra-high-efficiency, ultra-low-cost solar cells

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Abstract

Perovskite/silicon (Si) tandem solar cells (TSCs) continue to rapidly advance. To date, various Si solar cell technologies, such as an aluminium back surface field (Al-BSF), passivated emitter and rear contact (PERC), and heterojunction (HJT) have been explored as the bottom sub-cell in monolithic, 2-terminal (2-T) perovskite/Si TSCs. However, the majority have been built on HJT solar cells thanks to their high open-circuit voltages, largely exceeding 700 mV. They also feature the ease of electrical integration with the top cell due to the use of transparent conductive oxides (TCOs) as electrodes, where the optical shortcomings in HJTs of poor blue response are not as much of an issue for tandem cells. However, from an industrial perspective, currently HJT cells are less appealing due to concerns including the high cost, in particular the expensive low-temperature silver (Ag) pastes and depreciation of HJT-specific fabrication equipment. While Ag is currently used in the majority of mass-produced Si cells, the HJT architecture requires around 1–2 times higher Ag content than the PERC cells. Calculations indicate that no solar PV technology requiring indium (In) can be manufactured at scale sustainably. The current HJT design, for example, uses 200 nm of indium-doped tin oxide (ITO) (approximately 100 nm on each surface), which limits sustainable manufacturing capacity to less than 40 GW. In addition, the efficiency of HJTs degrades at temperatures above approximately 200 °C, thus placing a limiting temperature threshold on the materials and processing steps that can be used for optimizing the top cell in a tandem device. Techno-economic analysis has shown that despite their higher efficiency, the higher cost of HJT cells means that other Si bottom cell architectures could lead to a lower LCOE.

In this talk, I will present our work on how to achieve high efficiencies for perovskite/Si TSCs with Si bottom cells based on a poly-Si/Si dioxide (SiO₂) passivating contact (poly-Si cell) without silver or TCOs, fabricated using mass-production techniques. Meanwhile, I will introduce a novel low-absorption, dopant-free bilayer-structured hole transport layer (HTL) composed of ultra-thin poly(*N,N'*-bis-4-butylphenyl-*N,N'*-bisphenyl)benzidine (Poly-TPD) and 2,2',7,7'-tetra(*N,N*-di-*p*-tolyl)amino-9,9-spirobifluorene (Spiro-TTB) double layers developed for the perovskite top cell, which passivates the perovskite surface and enhances the near-interface conductivity, thus increasing the open-circuit voltage and fill factor. A power conversion efficiency of more than 29% was achieved, the highest for a perovskite/Si TSC based on poly-Si bottom cells and/or n-i-p perovskite top cells reported to date.

Solvothermal synthetic designs advance thermoelectric materials

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Solvothermal synthesis offers advantages such as simplicity and low cost, yet its potential in the design and application of thermoelectric materials remains underexplored. This report comprehensively summarizes our recent findings, showcasing advances in structuring thermoelectric materials through solvothermal synthesis to enhance both thermoelectric and mechanical performance. We discuss progress in synthesis techniques, characterization methods, thermoelectric performance enhancement, and potential applications. Additionally, we outline future prospects for developing solvothermal-based thermoelectric materials and devices across various application scenarios.

Spin-orbit electronics in Van der Waals heterostructures

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As an all-electrical scheme to generate, detect and manipulate spin current, the spin Hall effect has been heavily investigated as a primary route toward next-generation spintronic devices. Traditional spin Hall materials are mostly based on heavy metals, like Pt, W and Ta, that have strong spin-orbit coupling. However, the high symmetry and dimensionality of these materials make the control and optimization of spin Hall effect a major obstacle toward device applications.[1] In this talk, I will present our recent progress in studying the spin Hall effect in atomically thin 2D crystals. Relying on the symmetry breaking in 2D crystals, we broke the longstanding tradeoff between spin Hall angle and spin diffusion length in traditional spin Hall materials.[2] In addition, the 2D nature enables us to use electrostatic field to control the spin-charge conversion in a broad range. Finally, I will discuss how we use van der Waals heterostructures of 2D semimetal and 2D ferromagnets to achieve highly efficient interface spin transport and eventually a spin readout signal that is two orders of magnitudes higher than conventional 3D structures.[3] Our demonstrations prove the appealing potential of 2D spin Hall crystals as building block for highly efficient spintronic devices, including memory and logic devices.

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Zinc Depletion-Mediated Failure- Unveiling the Realistic Failure of Zn Anode

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Keywords: Aqueous Zn-ion batteries; testing protocol; Zn depletion

Abstract

Dendritic zinc electrodeposition-mediated short-circuiting is the predominant failure mode reported for aqueous zinc batteries. While the severity of zinc corrosion is gradually recognised, corrosion-mediated zinc depletion and corresponding failure is rarely discussed. By considering the important practical parameters- zinc reserve and electrolyte-to-capacity ratio- this study thoroughly examines corrosion-mediated zinc depletion and associated cell failure. Surprisingly, under high Zn utilization and thin separator, zinc depletion emerges as a more severe challenge than previously expected. Due to the existence of the second zinc electrode in the Zn-Zn cell, the symmetric setup significantly inflates the battery's lifespan. Conversely, the asymmetric setup accurately simulates zinc-starved conditions, accurately estimating both dendrite and corrosion-associated battery failure, which is consistent with full-cell cycling results. This study elucidates the reasons behind the performance gap between half-cells and full cells, offering an accurate testing protocol for Zn reversibility that will inform future research.

Passive Radiative Cooling Textiles

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Passive radiative cooling textiles have garnered significant attention for their potential to address critical energy and climate challenges [1–5]. By leveraging nanostructures and specialized material properties, these fabrics reflect incoming solar radiation while emitting thermal radiation through the atmospheric window into space. Fig. 2 presents a woven passive cooling nanoporous polyethylene (NanoPE) textile that we fabricated. Such textiles can achieve a skin temperature reduction of up to 3°C in indoor environments and 10°C in outdoor settings compared to conventional cotton. Radiative cooling textiles offer a compelling solution for maintaining thermal comfort in summer heat without electricity. Beyond personal comfort, they can enhance thermal regulation and prevent hyperthermia in diverse settings such as offices, homes, factories, sports, fieldwork, and medical applications. On a larger scale, these materials can be employed for rooftops and canopies, helping to cool the surrounding microclimate, including entire buildings. They have the potential to reduce global energy consumption for air-conditioning by up to 40%, equivalent to approximately 5% of total global energy use [1,3].

In this talk, we will review the initial development of radiative cooling textiles and highlight our recent progress. We will explore the fundamental principles of passive radiative cooling textiles, their fabrication methods, and strategies for performance optimization. Additionally, we will address the limitations of earlier cooling textiles, which rely on exotic materials such as specialized polymers and metals, making them impractical for mass-market adoption. In contrast, cotton stands out as a superior alternative due to its natural origin, affordability, comfort, biodegradability, breathability, aesthetic versatility, and compatibility with existing industrial processing chain. We will present our advancements in nano-engineering cotton to achieve effective radiative cooling.

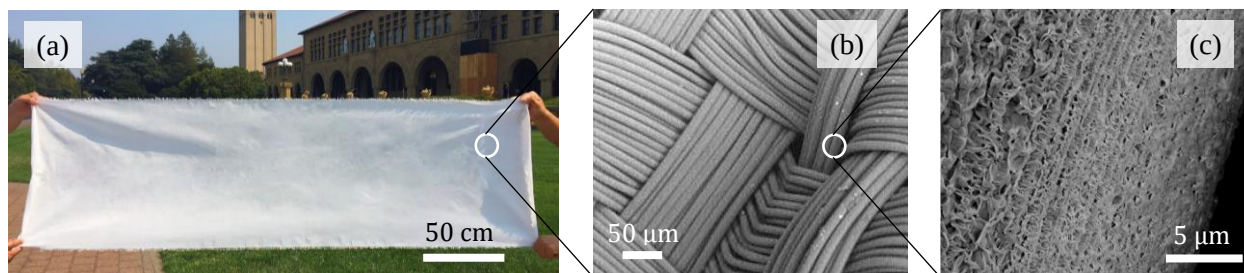


Fig. 2. Fabricated passive cooling NanoPE textile. (a) optical image, (b) SEM image showing woven structure, (c) SEM image of random nano pores in each fibre.

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Engineering Smarter Delivery Systems based on Self-Immolative Polymers.

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The use of polymeric materials for biomedical applications has generated intense interest in the last twenty years. While there have been some significant successes in this field, we still have limited polymeric materials used in clinical applications. One of the challenges with translating nanoparticles to clinical use is the many biological roadblocks that prevent successful delivery, [1,2] thus there remains a need to design smarter materials to migrate these barriers. This is especially important when we consider the use of emerging therapeutics such as nucleic acid. Self-immolative polymers have generated interest for the design of nanoparticle delivery systems as they can depolymerize in response to a range of biological stimuli and thus can be readily tuned to control the efficiency of therapeutic delivery.

Herein, we discuss the development of new stimuli-responsive delivery systems based on the self-immolative polymers of poly(ethyl glyoxylamide) (PGAm) and poly(lipoic acid) respectively. [3] In our work we have demonstrated that PGAm systems can be engineered to respond to a tunable pH range based on modifying the polymer backbone. These particles combine several advantages such as the ability to show pH triggered release of peptides and potential for endosomal escape. We have also developed delivery systems that can respond to a combination of pH and redox potential based on lipoic acid. These systems demonstrated successful transfection of plasmid DNA with over 80 % transfection efficiency. These studies indicate the potential of self-immolative nanoparticles to migrate inherent biological roadblocks for therapeutic delivery and thus provide useful materials for the future.

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Flat-band and tunable electronic states in two-dimensional Kagome systems

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Since the unique atomic arrangement of Kagome lattice usually lead to electronically destructive interference, namely flat band, many exotic physical phenomena have been explored promising for novel states in electronic topology, strong correlation, superconductivity etc. Most of the current research interest focus on the Kagome metals suggesting the desired emergence of Kagome semiconductors. Here we report several kinds of Kagome semiconductors with inorganic or organic frameworks. We predicted that the two-dimensional inorganic system has a rich variety of non-collinear magnetic structures, which determine their topological states of Kagome materials. Intriguingly, large Chern numbers can be obtained in noncollinear and noncoplanar magnetic structures leading to the quantum anomalous Hall effect and the quantum spin Hall effect even if the time-reversal symmetry is broken [1]. We further discovered that achiral conjugated organic molecules can form a chiral Kagome lattice, which is completely derived from the intermolecular electronic state without atomic occupation. These results were confirmed by density functional theory calculations and scanning tunneling microscope experiments [2]. Lastly the Kagome lattice with strong spin-orbit coupling is selective to the chirality of the light field, and its spin channel and chirality of the light field will be strongly coupled, which can transform the non-local dispersive energy band in real space into highly localized topological flat bands, which are expected to realize high-temperature fractional quantum Hall effect states [3]. The use of periodic light fields to tune the spin topological states of inorganic and organic systems and their strong correlation effects is of great significance for realizing the novel topological states in Kagome materials.

Keywords: Kagome lattice, topological states, charge density of wave, conjugated organic molecules, spin-orbit coupling, light-matter interaction

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Structure Design of Polymer Electrolyte for Solid-state Lithium Batteries

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Solid-state batteries, with their potential for high energy density and improved safety, represent a significant direction in electrochemical energy storage devices. Among the various solid-state electrolytes, solid-state polymer electrolytes (SPEs) are lightweight, low-cost, more flexible, and easier to process, which contributes to higher energy densities and scalable production for solid-state batteries. The structure of the polymer materials determines the transport behavior of the lithium ions in the polymers and thus affect the performance of the energy storage devices. To address the low ionic conductivity of polymer electrolytes, we introduced succinonitrile into the PEO main chain to optimize the coordination environment for lithium ions and the relaxation ability of polymer chain segments, which led to the rapid transport of lithium ions in PEO-based electrolytes [1,2]. In addition, a general solidified localized high-concentration electrolyte strategy was proposed to achieve solid-state lithium metal batteries that can operate in a wide temperature range and excellent fast charge/fast discharge capability [3]. These strategies provide new ideas for polymer applications in electrochemical energy storage and for improving the performance of solid-state batteries.

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The pathway towards high efficiency high bandgap $\text{Cu}_2\text{ZnSnS}_4$ solar cells

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High bandgap sulfide kesterite $\text{Cu}_2\text{ZnSnS}_4$ (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 interface^[3-5] and kesterite/back contact interface^[6] are the three main regions have been focused. The future development direction and insight will also be touched.

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Carbon-based Hybrid Catalytic-Protective Overlayer for Efficient and Stable Kesterite Photocathode for Solar Hydrogen Production

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Abstract

Developing stable and efficient photocathodes with low-cost components is crucial for advancing the commercialization of photoelectrochemical (PEC) water splitting devices, specifically for hydrogen evolution reaction (HER). In this work, we present a cost-effective solution-processed hybrid layer composed of fullerene (C60) grafted onto nitrogen and sulfur-doped graphene (NSG), which serves as a catalytic-protective overlayer for the earth-abundant kesterite $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ (CZTSSe) photocathode in acidic environments. The resulting CZTSSe/CdS/C60-NSG/Pt photocathode shows an impressive current density of 27.7 mA/cm² at 0 V reversible hydrogen electrode (RHE), a half-cell solar-to-hydrogen efficiency exceeding 3%, an onset potential of 0.51 V and excellent durability, retaining 80% of initial current density after 10 h of operation. Additionally, the band alignment of the CZTSSe/CdS/C60-NSG photocathode is optimized to facilitate charge separation and transfer compared to the CZTSSe/CdS structure alone. Spectroscopic analyses and density functional theory (DFT) studies indicate that the C60-NSG hybrid layer improves carrier lifetime, facilitate efficient charge transfer, and provides catalytic sites with Gibbs free energy close to thermoneutral for adsorbed H species, leading to superior HER activity and stability. Our findings highlight the potential of employing a cost-effective solution-processed ‘carbon-based’ hybrid catalytic-protective layer on photocathodes for sustainable hydrogen production.

Quantum Material Research Capabilities at the Australian Synchrotron

Anton Tadich

Australian Synchrotron, ANSTO, Australia

Condensed matter systems exhibiting exotic, emergent quantum effects in reduced dimensions and scale (“quantum materials”) offer exciting platforms for next-generation electronics, sensing, quantum computing, and more. Understanding the atomic, chemical and electronic structure at a fundamental level is crucial for the development and implementation of this promising technology. This presentation will begin with an introduction to the Australian Synchrotron, providing a broad overview of the range of techniques that are available at the facility for characterising quantum materials. Some examples from the beamlines in quantum materials and semiconductor research will be given. The latter half of the presentation will focus on the soft X-ray spectroscopy beamline. With a photon energy range of 82 – 2500 eV and full polarisation control of the x-rays, the beamline features three experimental stations capable of performing Angle-Resolved Photoelectron Spectroscopy (ARPES), X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS). All three techniques are supported by a wide range of sample preparation tools and offline characterisation methods. Recent investigations of various quantum material systems are presented, covering 2D and 3D topological insulators/semimetals, 2D materials (graphene, black phosphorus) and diamond surface functionalization.

Manipulating FA-based Perovskite Growth for High-efficiency Solar Cells

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The past 15 years have seen dramatic increases in the performance of perovskite solar cells (PSCs) with certified efficiencies on par with crystalline silicon solar cells. Among them, formamidinium lead iodide (FAPbI₃) is the most promising configuration to approach the Shockley-Queisser limit due to its bandgap (~1.48 eV) close to the ideal one. The key challenge for FA-based PSCs is to obtain high-quality polycrystalline films with stable black α phase. In this regard, I'll show you three kinds of methodology to manipulate FAPbI₃ perovskite growth upon sequential deposition to obtain high-quality polycrystalline films with low defects [refs. 1-3]. Consequently, the resultant perovskite solar cells yielded substantial power conversion efficiencies with improved stability.

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Polymerizable Eutectics for the Preparation of Functional Materials

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In this presentation I will discuss our recent work on the design of various classes of polymeric materials from what we term “polymerizable eutectics.” Polymerizable eutectics are a sub-class of deep eutectic solvents (DES), which have gained significant attention in recent decades due to their appealing physical and chemical properties as alternatives to traditional organic solvents. Polymerizable eutectics comprise of one (or more) monomer, either acting as hydrogen bond donor or acceptor, mixed with another species to generate a stable liquid at room temperature, often from high melting point starting materials.

We have prepared thermoresponsive hydrogels, porous monoliths, block copolymers and photocurable resins based on the free-radical or controlled-radical polymerization of polymerizable eutectics based on acrylamides (e.g. N-isopropylacrylamide, acrylamide) and various other (meth)acrylates. Low melting point mixtures were formed by mixing these monomers with quaternary ammonium salts (e.g. choline chloride) in specific ratios that were characterised by 1D/2D NMR, DSC and thermogravimetric analysis. This platform was used as the basis for direct polymerization in the absence of traditional solvents. Hydrogels prepared from such eutectics showed greatly enhanced polymerization kinetics compared to the equivalent synthesis in water, in addition to displaying greater mechanical strength due to an increase in cross-linking density. Thermoresponsive macroporous polymer monoliths were prepared from high internal phase emulsions (HIPEs) where the eutectic was the polymerizable continuous phase, which displayed remarkably different internal morphologies and mechanical properties compared to those made in water. Lastly, we have shown that the rapid curing of these systems under UV light makes them ideal candidates for photopolymerization, including stereolithography 3D printing.

Selective-Area Growth of Vertical III-V Nanowires on Si and Transistor Applications

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Difficult issue for achieving ultralow-power integrated circuits (ICs) is lowering supply voltage of field-effect transistors (FETs) while overcoming physical limitation of subthreshold slope ($SS = 2.3 k_B T/q = 60 \text{ mV/dec}$). This limitation suppresses further scaling of the power consumption even if a gate-all-around (GAA) structures and III-V/Ge channels are implemented in near future. The steep-slope transistors such as tunnel FETs (TFETs) and negative-capacitance FETs have therefore been proposed to overcome the limitation. The TFETs are most promising switching devices because of scalability for lower SS than 60 mV/dec and best compatibility with conventional integration process. However, there are some difficulties in decreasing SS while increasing on-state current as high as that of conventional FETs. Recently, we have successfully integrated vertical III-V nanowires on Si substrates by selective-area growth [1]. The important point for the heterogeneous integration was to modify the initial Si or Ge surfaces to (111)B-polar. And we demonstrated high-performance III-V NW-based vertical FETs using modulation doped core-multishell structures [2]. Beside the application, we proposed a new tunnel junction based on III-V/Si interface which is formed by selective-area growth of vertical III-V nanowires (NWs) on Si, and demonstrated vertical TFETs with steep SS [3]. This new tunnel junctions can inherently forms abrupt heterojunction regardless of precise doping because the band discontinuity is determined only by the offset of each III-V and Si. Thus, good gate-electrostatic and depletion-layer controlling are defined only by the III-V channel region.

In this presentation we report on recent progresses in these heterogenous integrations of III-V nanowires on Si and SOI substrates, and device applications such as the vertical III-V NW FETs on Si or SOI, and steep-slope TFETs using the III-V NW/Si heterojunctions. In TFET application, we present new approach of increasing tunneling current which is inherently low current. The new TFET using III-V NW/Si junction demonstrate rapid current enhancement and exhibit very high transconductance efficiency which was much higher than the physical limitation of Si MOSFET-based analog integrated circuits.

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Dynamic Chalcogen Squares for Material and Topological Control over Macromolecules

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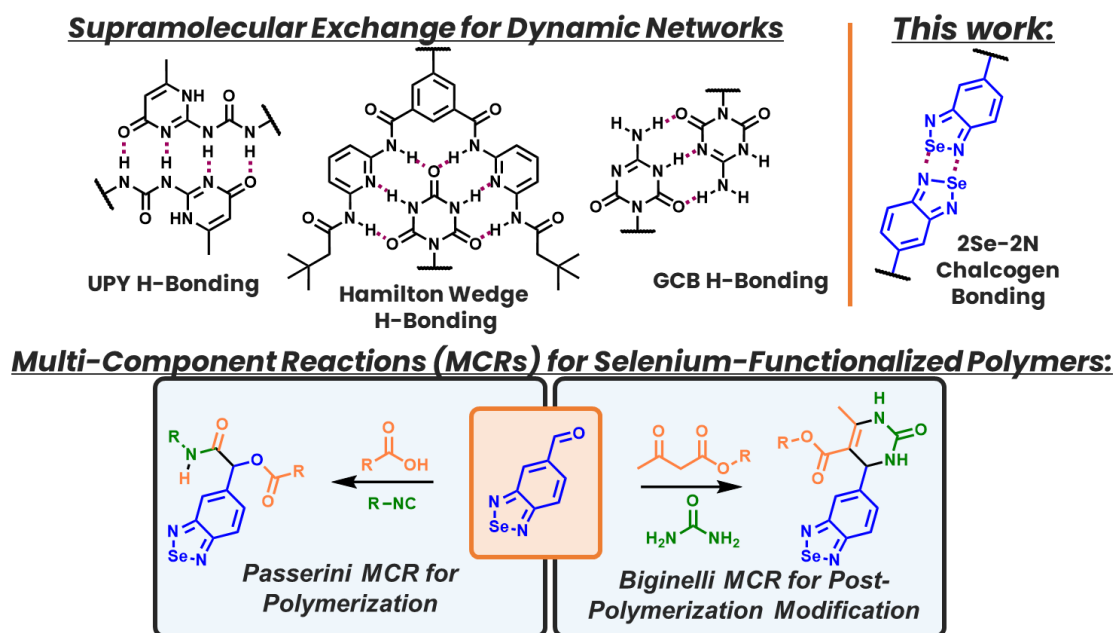
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Herein we introduce chalcogen squares via selenadiazole motifs as a new class of dynamic supramolecular bonding interactions for the modification and control of soft matter materials. We showcase selenadiazole motifs in supramolecular networks of varying primary chain length prepared through polymerization using tandem step-growth/Passerini multicomponent reactions (MCRs). Compared to controls lacking the selenadiazole motif, these networks display increased glass transition temperatures and moduli due to the chalcogen bonding linkages formed between chains. These elastomeric networks were shown to autonomously heal at room temperature, retaining up to 83 % of the ultimate tensile strength. Lastly, we use post-polymerization modification via the Biginelli MCR to add selenadiazole motifs to narrowly dispersed polymers for controlled topology in solution. Chalcogen squares via selenadiazoles introduce an exciting exchange mechanism to the realm of dynamic materials. ^[1]



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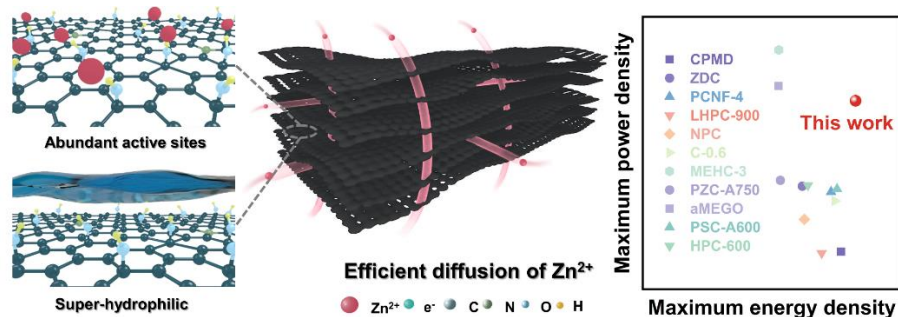
Synthesis of Advanced Electrode Materials for Zinc based Energy Storage Devices

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Aqueous zinc-based energy storage devices (AZDs) including batteries and supercapacitors are advantageous with their remarkable safety, abundant Zn reserve, cost-effectiveness, and relatively high energy density. However, AZDs still face issues like Zn anode dendrite growth and limited cathode capacity. We critically examine the recent progress of various advanced materials for electrochemical energy storage applications including AZDs.[1-2] Moreover, we present a facile method for fabricating a robust $\text{CoSe}_2@\text{Ni}_3\text{Se}_4@\text{Ni}(\text{OH})_2$ superstructure nanoarray (CNSNA) as an alkaline Zn battery (AZB) cathode.[3] The sophisticated design enables structural stability and abundant active surface sites for efficient charge storage. The corresponding AZB based on CNSNA demonstrated an extraordinarily high energy density of $516.58 \text{ Wh kg}^{-1}$. We also employed a two-dimensional (2D) metal-organic framework (MOF) nanosheet precursor to fabricate an ultra-thin N-doped oxygen-rich porous carbon nanosheet (A-NOCNS) for zinc-ion hybrid supercapacitor (ZIHSC) applications.[4] The as-prepared A-NOCNS has an atomically thin thickness of only a. 2.5 nm, a high surface area, and a hierarchical porous structure with a microporous pore domain, which provides abundant surface active sites, fast ion diffusion channels, and efficient charge transport paths. Moreover, the uniform doping of N and rich O atoms provides extra redox capacitance, as well as super-hydrophilic properties. Consequently, the ZIHSC based on the A-NOCNS delivers exceptional energy and power densities ($162.88 \text{ Wh kg}^{-1}$ and 28.43 kW kg^{-1} , respectively), and long-term cycling stability (90.23% after 20,000 cycles at 10 A g^{-1}). Our recent research findings may facilitate the rapid development of advanced AZDs.



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Doping Effects on Structural, Electronic, and Oxygen Evolution Reaction Properties of Perovskite Oxide Thin Films

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Electrochemical water splitting is a promising clean technology for generating hydrogen gas from water, but its practical use is largely hindered by the anodic oxygen evolution reaction (OER), which suffers from slow reaction kinetics associated with its multiple proton-coupled electron transfer reactions. To address this challenge, there is a critical need for the development of efficient and stable electrocatalysts. Earth-abundant transition metal perovskite (ABO₃) oxides, with their high compositional flexibility and electronic tunability, offer a compelling alternative to benchmark OER electrocatalysts based on platinum group elements. In this talk, I will showcase how the epitaxial synthesis of complex oxide thin films enables precise control over material composition and structure, allowing the establishment of key structure–property–stability relationships.^[1,2] Using nickelate thin films as model systems,^[3–6] I will illustrate how epitaxial design facilitates testing of different hypotheses and proposed performance descriptors, and provides a platform for formulating new design principles in electrocatalysis. I will begin by introducing advanced epitaxial growth techniques that allow atomic-level manipulation of perovskite thin films, followed by a discussion on how various doping strategies — including A-site, B-site, and anion doping, as well as high-entropy effect — affect structural and electronic properties such as oxygen vacancy formation, transition metal 3d and oxygen 2p orbital hybridization, and surface binding energies. These doping-induced changes have a direct impact on OER performance. Key insights from advanced experimental techniques such as X-ray absorption spectroscopy (XAS) and time-of-flight secondary ion mass spectrometry (TOF-SIMS), complemented by theoretical modeling, offer a deeper understanding of how doping affects the material's structural and electronic properties. This work highlights the essential role of doping in tailoring the structural and electronic features of perovskite oxides, paving the way for the optimization of these materials for enhanced catalytic performance in renewable energy applications.

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Controllable Synthesis of 2D Metal Nitrides and Their Heterostructures

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The synthesis and design of two-dimensional (2D) materials and their heterostructures have become critical in advancing applications in catalysis, energy storage, and photothermal conversion. In recent years, various techniques such as chemical vapor deposition (CVD) and template-assisted methods have enabled the controllable synthesis of materials like Nb₄N₅, MoN, and other metal nitride heterostructures.

Firstly, we explored the rapid growth of hexagonal MoN nanosheets using a CVD method on a liquid copper substrate, achieving crystal thicknesses down to 1 nm within minutes. These MoN nanosheets exhibit high catalytic efficiency for hydrogen evolution reactions (HER), attributed to their exposed active surface sites and excellent electron transport properties.^[1]

Similarly, higher-metal nitrides, including Mo₅N₆ and Nb₄N₅, have shown promise in solar steam generation applications due to their enhanced photothermal properties. Using an amine-functionalized precursor strategy, we prepared the Mo₅N₆ and the MoS₂-Mo₅N₆ nanosheets with superior photothermal conversion efficiency compared to traditional MoS₂.^[2-5] These higher-metal nitrides and heterostructures also demonstrated remarkable chemical stability and potential for scalable production.

By tuning reaction conditions such as gas ratios, temperature, and precursor materials, we can precisely control the morphology and thickness of 2D materials.^[6] These studies highlight the advancements in scalable, controllable synthesis of 2D metal nitrides, which offer unique properties for electrochemical, photothermal, and catalytic applications. The development of these methods opens new pathways for the creation of high-performance heterostructures, pushing the boundaries of material science.

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Two Strategies to Prepare MXene Based Flame Retardant Composites

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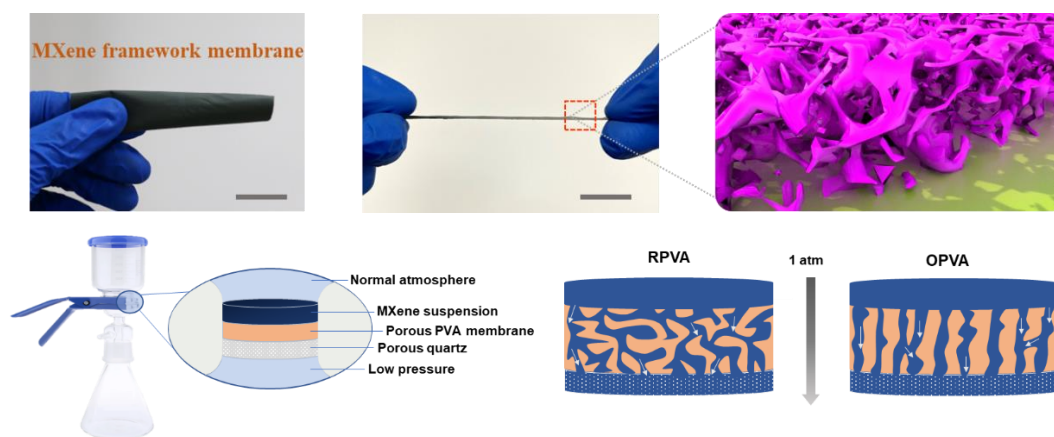
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Abstract

Nowadays, highly flexible, ultrathin, and multifunctional polymer composites are exceptionally desirable for various applications. While the traditional nanocomposites blending remains the mainstream method and results in poor dispersion and properties. For MXene nanosheets showing hydrophilic feature, it can be widely used in hydrophilic polymer composites, but quite difficult to be employed in hydrophobic polymer composites. Another critical issue is that it needs a high loading of MXene to realise high-performance polymer composites due to the poor connectivity of MXene inside the substrates. This presentation will introduce two strategies respectively aerogel method and template method to employ MXene nanosheets in hydrophobic polymer composites [1] and construct electrically conductive networks inside polymer composite with a low loading MXene [2]. For the aerogel method, it's a good way to prepare porous MXene-based aerogel first and then incorporate it with targeted hydrophobic polymer resins. The well distribution of MXene networks can help promote the flame retardancy of polymer composites. In terms of template method, the polymer template can result in connected MXene network inside of the polymer matrix that can impart with outstanding fire resistance, good electrical conductivity, and EMI shielding performance. The shortage of this method is that the preparation process is relatively complex and has high requirement of the condition.

Keywords: MXene; Conductive networks; Flame retardancy; Fire safety; Polymer composites.



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Rational Catalyst Design for CO₂ Electrochemical Reduction Reaction

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Electrochemical CO₂ reduction (CO₂RR) offers a promising route for converting CO₂ into valuable chemicals and fuels using renewable electricity [1]. However, significant challenges remain in terms of product selectivity, energy efficiency, and long-term stability, particularly when using industrially-relevant CO₂ sources. This talk will present recent advancements in CO₂RR, drawing from several cutting-edge studies that address these challenges from multiple angles.

In this talk, we will first introduce a general computational framework for catalyst design [2]. Then, we will use density functional theory (DFT) calculations to understand the reaction pathways of CO₂RR to multiple products. The reaction barriers and enthalpy changes are calculated for the elementary steps considered in all the pathways on Cu(100). We will then introduce the selectivity determinants based on microkinetic modelling.

Furthermore, we will discuss novel catalyst designs, including cationic-group-functionalized copper catalysts that enable stable acidic CO₂ electrolysis with high selectivity towards multi-carbon products [3]. The role of the catalyst-electrolyte interface in promoting CO₂ activation while suppressing competing reactions will be examined. We'll also explore system-level innovations, such as proton-exchange membrane electrolyzers that achieve durable CO₂ conversion to formic acid using recycled lead catalysts [4].

Furthermore, we'll address the critical issue of catalyst poisoning by trace impurities in industrial CO₂ streams, presenting strategies to improve SO₂ tolerance through rational catalyst and electrode design⁵. The talk will highlight how these advances, combining computational chemistry and experiments, collectively push the boundaries of CO₂RR performance.

By integrating insights from catalyst development, reaction mechanisms, and electrolyser engineering, this work demonstrates significant progress towards making CO₂ electrolysis a viable technology for large-scale carbon utilization and renewable fuel production.

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Designing Metal Nanowires for Flexible and Wearable Applications

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Metal nanowires have been considered as a promising alternative material to traditional indium tin oxide (ITO) for transparent electronics owing to their excellent electrical conductivity and good optical performance. However, they suffer from low mechanical property and poor thermal and electrical stability, limiting their applications in next-generation electronics. In this work, silver nanowires (AgNWs) and copper nanowires (CuNWs) have been synthesized via facile solution processes, and structural-dependent characteristics have been demonstrated. To boost their overall performance, various strategies have been employed, such as engineering the NW structure, constructing core-shell architectures, and introducing surface coating. The NWs can be easily deposited as films or patterned with a high resolution by combining inkjet printing and adhesion manipulation. The resultant NWs-based devices show superior performance and good stability, making them suitable for diverse flexible and wearable applications, such as transparent heaters/electrodes, strain/pressure sensing, and humidity monitoring. With the assistance of machine learning, the tailored NWs can effectively recognize morse code and breathing patterns, which are promising for human-machine interaction.

The catalytic and substrate role of carbon nanotube in electrocatalytic reactions

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As an important member of the carbon material family, carbon nanotubes (CNTs) have been extensively utilized in electrocatalysis as catalysts or catalyst substrates due to their large surface area, good electrical conductivity, and versatile surface chemistry. Here, we demonstrate that the geometry and surface chemistry of CNT are critical to their roles as both catalysts and support. For example, the CNT curvature, or diameter, could determine its oxygen reduction reaction (ORR) activity after mild oxidation. Theoretical and experimental results found that CNTs of smaller diameter could provide higher selectivity and activity towards the two-electron transferred ORR pathway, e.g., an oxidized CNT with an 8 nm diameter could deliver an H₂O₂ Faradaic efficiency >85%, and an impressive mass activity of 161 A g⁻¹ at 0.65 V, making one of the best carbon-based catalysts reported recently. Moreover, we also show that the surface chemistry of the CNT, particularly the density of oxygenous functional groups, could substantially impact the ORR and CO₂ reduction reaction performance when used as a substrate to accommodate catalytic active cobalt phthalocyanine molecules. These findings highlight the importance of controlling the geometry and surface chemistry of CNTs towards high-performance electrochemical reactions.

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Functional organic materials to construct high-energy and stable electrode

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Functional organic materials (FOMs) are crucial for constructing high-energy and stable electrode for rechargeable metal ion batteries. FOMs with redox-active groups such as C=O or C=N bonds enable multiple electrons transfer reactions, offering the high-capacity electrode for mono/multivalent batteries. Additionally, organic molecules containing heteroatomic groups can act as effective electrolyte additives, helping to stabilize electrodes by ensuring uniform deposition and stripping processes, and forming a strong solid electrolyte interphase (SEI) or cathode electrolyte interphase (CEI) on the electrode surface. In our study, we designed, synthesized, and applied a series of FOMs as high-capacity electrode materials and functional electrolyte additives for metal-ion batteries. [1-5] We will discuss the design principles and the related energy storage mechanisms in detail. The use of FOMs in these batteries enhances their energy density and cycling stability, offering significant improvements for future energy storage technologies.

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Elastic Conductive Biopolymer Nanocomposites for Wearable Sensors

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Flexible and stretchable strain sensors have recently gained significant attention for their potential in applications such as health monitoring, electronic skin, human-machine interfaces, and soft robotics [1]. Typically, these sensors are made from elastic polymers like polydimethylsiloxane (PDMS) and polyurethane, combined with conductive nanomaterials like silver nanowires, MXene, carbon nanofibers (CNFs), and graphene [2-4]. Due to their outstanding flexibility, these sensors can be seamlessly attached to curved surfaces (e.g., human body or clothing), facilitating real-time tracking of movements and health indicators. However, most of these sensors are made from non-biodegradable synthetic polymers. As these sensors become more widely adopted, the accumulation of electronic waste from sensor replacements and upgrades could present a substantial ecological and environmental concern.

In this work, we present a new type of flexible, stretchable, and bio-disintegrable piezoresistive strain sensors based on elastic biopolymers (i.e., cellulose, starch) [2-4]. The sodium carboxymethyl cellulose (NaCMC) was chosen as the natural polymer matrix because it is water-soluble, which makes it easy to process. To develop thin films with high elastic stretchability, NaCMC was physically modified by adding plasticizers (i.e., glycerol) and other polymers such as starch and polyvinyl alcohol (PVA). The additives contain abundant hydroxyl groups and form hydrogen bonds with NaCMC to disrupt the strong hydrogen bonds inside NaCMC, resulting in highly flexible and stretchable thin films. The thin films were then used as the substrate, onto which conductive nanohybrids of CNFs and Au or CNFs and poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) were deposited. The effects of the polymer blend composition (e.g., glycerol, polymer additive content) on the mechanical and the thickness of conductive coating on the electromechanical properties of the sensors were thoroughly investigated. The resultant bilayer conductive polymer nanocomposites exhibit excellent elastic stretchability (failure strain up to ~330%), low hysteresis (5.74% at the second cycle) when subjected to 50% cyclic strain, and durable piezoresistivity with a maximum gauge factor of 1.7. Lastly, the potential applications of the sensors in joint bending detection as well as physiological sign (heart rate, respiration rate) measurement have been demonstrated.

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Solar-Powered Methanol Conversion for On-Demand Hydrogen Production

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Hydrogen as a green energy carrier promises a zero-emission and sustainable future for human society. However, the low density and high explosiveness of hydrogen gas make it challenging to store and transport safely and cost-effectively in large commercial quantities. Methanol has been recommended as one of the most promising liquid hydrogen carriers because of its low cost, easy production from a wide range of sources, liquid phase at ambient conditions, and existed manufacturing and transporting foundations. Solar-driven photocatalytic methanol dehydrogenation holds great promise to release hydrogen from methanol. This approach can achieve the conversion of methanol to hydrogen using renewable solar energy and enable instant hydrogen generation and frequent on-off operating cycles for on-demand hydrogen production using a very simple photocatalytic system. Nevertheless, the purity of produced hydrogen is a concern for various applications, due to the formation of CO, CO₂ and CH₄ by-products. For example, a hydrogen purity of $\geq 99.97\%$ is generally required for fuel cell vehicles to avoid the poison of catalysts. Therefore, the delicate design of photocatalysts is highly desirable to suppress the formation of gaseous carbon by-products for photocatalytic methanol dehydrogenation. In our works, we rationally engineered functional nanomaterials and explored their performance for photocatalytic methanol dehydrogenation, including 1) the design of single-atom catalysts; 2) the understanding of the reaction mechanism for methanol dehydrogenation; and 3) the development of liquid-phase and gas-phase reaction systems. A high solar-to-hydrogen (STH) conversion efficiency of 2.3% was achieved and the feasibility of directly harvesting sunlight energy for on-demand H₂ production from methanol was further demonstrated.

Zero-Strain Electrode Materials for Sodium-Ion Batteries

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Sodium-ion batteries (SIBs) are considered a complementary or even an alternative energy storage technology to lithium-ion batteries (LIBs). Fundamental challenges, such as sluggish charge transport kinetics, short cycling lifespan, and low energy density, hinder the current technological development of SIBs. Electrode materials hold the key to any success in commercialising SIBs. The past decade has witnessed rapid advances in the design and synthesis of high theoretical capacity anode materials, such as metal/alloys, metal oxides/dichalcogenides, phosphorous/phosphides, *etc.*, for SIBs. These candidates, however, face challenges such as significant volume expansion upon Na ion insertion, limiting their electrochemical reversibility and cycling stability, and sluggish sodiation kinetics, resulting in inferior rate capability. Electrode materials with high specific capacity and zero-strain properties have shown the potential to improve the electrochemical of SIBs but with long-term stable cycling, even under extreme temperature environments. This abstract will present our recent research results on developing zero-strain anode materials of titanium-based oxides and hard carbons for SIBs, including the material structural design and synthesis, in situ characterisations, and electrochemical properties.

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Pick-and-place transfer of arbitrary-metal electrodes for scalable van der Waals device fabrication

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Van der Waals electrode integration is a promising strategy to create near-perfect interfaces between metals and two-dimensional materials, with advantages such as eliminating Fermi-level pinning and reducing contact resistance.^[1] However, the lack of a simple, generalizable pick-and-place transfer technology has greatly hampered the wide use of this technique. We demonstrate the pick-and-place transfer of pre-fabricated electrodes from reusable polished hydrogenated diamond substrates without the use of any sacrificial layers^[2,3] due to the inherent low-energy and dangling-bond-free nature of hydrogenated diamond surface. The technique enables transfer of arbitrary metal electrodes and electrode array, as demonstrated by successful transfer of eight different elemental metals with work functions ranging from 4.22 to 5.65 eV. We also demonstrate the electrode array transfer for large-scale device fabrication. The mechanical transfer of metal electrodes from diamond onto van der Waals materials creates atomically smooth interfaces with no interstitial impurities or disorder, as observed with cross-sectional high-resolution transmission electron microscopy and energy-dispersive X-ray spectroscopy. As a demonstration of its device application, we use the diamond-transfer technique to create metal contacts to monolayer transition metal dichalcogenide semiconductors with high-work-function Pd, low-work-function Ti, and semi metal Bi to create *n*- and *p*-type field-effect transistors with low Schottky barrier heights. We also extend this technology to air-sensitive materials (trilayer 1T' WTe₂) and other applications such as scalable ambipolar transistors Schottky diodes and optoelectronics. This highly reliable and reproducible technology paves the way for new device architectures and high-performance devices as well as exploring the emergent physics.

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Nano-strategy of Targeting at Embryonic Trophoblast Cells Using CuO Nanoparticles for Female Contraception

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Effective contraceptives have been comprehensively adopted by women to prevent the negative consequences of unintended pregnancy for women, families, and societies. With great contributions of traditional hormonal drugs and Intra-Uterine Devices (IUDs) to effective female contraception by inhibiting ovulation and deactivating sperm, their long-standing side effects on hormonal homeostasis and reproductive organs for females remain concerns. Herein, we proposed a nano-strategy for female contraceptive, inducing embryonic trophoblast cell death using nanoparticles to prevent embryo implantation. Cupric oxide nanoparticles (CuO NPs) were adopted in this work to verify the feasibility of the nano-strategy and its contraceptive efficacy. We carried out the in vitro assessment on the interaction of CuO NPs with trophoblast cells using the HTR8/SVneo cell line. The results showed that the CuO NPs were able to be preferably uptake into cells and induced cell damage via a variety of pathways including oxidative stress, mitochondrial damage, DNA damage, and cell cycle arrest to induce cell death of apoptosis, ferroptosis, and cuproptosis. Moreover, the key regulatory processes and the key genes for cell damage and cell death caused by CuO NPs were revealed by RNA-Seq. We also conducted in vivo experiments using a rat model to examine the contraceptive efficacy of both the bare CuO NPs and the CuO/thermosensitive hydrogel nanocomposite. The results demonstrated that the CuO NPs were highly effective for contraceptive. There was no sign of disrupting the homeostasis of copper and hormone, or causing inflammation and organ damage in vivo. In all, this nano-strategy exhibited huge potential for contraceptive development with high biosafety, efficacy, clinical translation and non-hormonal style and on-demand for women.

Liquid Metal Electrocatalyst for Direct Ethanol Fuel Cells (DEFCs)

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Developing efficient and durable electrocatalysts for ethanol electrooxidation is crucial for the development of direct ethanol fuel cell (DEFC) technology. Liquid metals are proved to be capable of providing intriguing route to access atomically dispersed metal atoms and maximize their utilization efficiency.[1] Here, we demonstrate that platinum-gallium (Pt-Ga) liquid metal nanodroplets with a low loading of Pt (~0.5 wt%) can serve as an efficient electrocatalyst to drive both ethanol oxidation and oxygen reduction reaction (ORR). Machine learning neural networks have been employed to formulate a low-concentration alkaline electrolyte to allow the liquid metal electrodes to demonstrate remarkable activity. Impressively, a mass activity as high as 13.47 A mg_{Pt}⁻¹ was achieved from the PtGa catalysts towards ethanol oxidation. Computational studies (DFT modelling) further revealed the reaction mechanism and highlights the significance of alloying Pt with Ga, i.e., presence of both Ga and Ga₂O₃ on the catalyst surface led to energetically favorable pathways for the oxidation process. The findings hold great promise for the future development of high-performance alcohol fuel cells.

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Advanced 2D Perovskite nanoplatelets in Energy Harvesting and Conversion Applications

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Two-dimensional (2D) perovskite nanoplatelets (NPLs) exhibit remarkable properties, such as a large Stokes shift and high photoluminescence quantum yield (PLQY). The colloidal nature of layered 2D perovskites offers tunable Stokes shift and enhanced PLQY through the control of organic cations and particle sizes, making them highly suitable as absorbers and emitters in down-conversion applications. Therefore, we incorporated an ultrathin layer of 2D NPLs-poly(methyl methacrylate) (PMMA) into semitransparent perovskite solar cells (ST-PSCs). The 2D NPLs demonstrated exceptional down-conversion ability, effectively transforming UV-blue light into visible light, thus enhancing photon absorption by the perovskite layer. This led to a significant increase in short-circuit current density (J_{sc}), resulting in champion power conversion efficiencies (PCEs) of 14.26% and 10.65% for devices with average visible transmittances (AVT) of 19.4% and 26.9%, respectively.^[1] In addition, in the field of piezoelectric nanogenerators (PENGs), 2D perovskite NPLs can serve as efficient fillers in the polyvinylidene fluoride (PVDF) matrix due to the polarization and centro-symmetry disruption of PbX_6 pyramids. The unpolarized 2D PSK NPLs@PVDF-based PENGs demonstrated the highest piezoelectric outputs, achieving an unprecedented voltage of 54.2 V, the highest reported for unpoled perovskite@PVDF-based PENGs to date.

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Focused Ion Beam sample preparation for Atom Probe Tomography

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In modern solid materials characterization, focused ion beam (FIB) lift-out is an essential technique for fabricating small-scale specimens for transmission electron microscopy (TEM) 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 (ROI) 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 for sample preparation.

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Advanced Hybrid Membrane for Vanadium Redox Flow Battery

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The application of vanadium redox flow batteries (VRFBs) has encountered challenges because the most commonly used commercial membrane (perfluorinated sulfonic acid, PFSA) has severe vanadium ion permeation, which yields poor stability of the battery. Nanomaterial modification is one of the effective ways to enhance membranes performance. By incorporating nanomaterials of these different dimensions (0D, 1D, and 2D) into the membrane matrix to optimize ionic conductivity and selectivity while minimizing vanadium ion crossover. The addition of nanomaterials not only improves the stability of the membrane and enhances its mechanical strength, but also provides more transport channels for protons. The composite membranes not only improved the electrochemical performance of the VRFBs, but also extended their operational life, demonstrating the potential of nanomaterial hybrid membranes for the development of VRFBs.

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Engineered Catalysts for Green Hydrogen Peroxide Production

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Photocatalysis hydrogen peroxide (H₂O₂) production has gained broad research attention since it is a potentially viable route for “green” on-site H₂O₂ manufacturing from just water and oxygen using renewable solar energy^{1,2}. In the past decade, stunning progress has been made. However, efficient photocatalysts are still in need to push the current boundaries of H₂O₂ production in terms of generation rate and product concentration³. Besides, a fit-for-purpose application is needed to demonstrate its practical use. In this presentation, we will talk about our recent works on the rational design of photocatalysts for improved H₂O₂ production⁴⁻⁶. Additionally, the application for disinfection of bacteria in water will also be covered. It is expected to provide insights on designing photocatalysts with judicious structures and function for environmental applications via green photocatalysis process.

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Short Biography

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Two-dimensional hexagonal germanium oxide- A wide bandgap semiconductor for next Gen electronics

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The compelling demand for next-generation electronic system drives the new material and device advances. Given the distinct physical properties of derived from the reduced geometry of 2D layers, they have been recognized to lead the roadmap for complementary metal-oxide-semiconductor (CMOS) technology. Though there has been significant 2D-enabled new material research and device concepts, the material exhibits both ultrahigh carrier mobility and wide bandgap has yet been reported so far. Here, we artificially created 2D Germanium oxide with planar layered hexagonal structure from Ge surface. The obtained h-GeO₂ possesses a wide bandgap of approximately 3 eV. The field-effect transistor (FET) device based on few layered h-GeO₂ achieved a significant mobility at hole side up to 24,700 cm²V⁻¹s⁻¹. The theoretical simulation has revealed its band hybridization which allows a distinct dual hopping path for electrons and a largely improved carrier mobility. The outcome suggests advancement in new material and device mechanisms with promising potential for post Moore nanoelectronics.

Bifunctional Electrocatalysts for Hydrogen Electrolyser

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Hydrogen is a highly efficient zero-emission energy carrier, characterized by an energy density of 120 MJ/kg, surpassing that of conventional fuels such as liquefied natural gas (54.4 MJ/kg), coal (27 MJ/kg), and automotive diesel (45.6 MJ/kg).¹ Electrochemical water splitting presents a viable method for producing high-purity green hydrogen, contributing significantly to global decarbonization efforts.² The effectiveness of water electrolysis is contingent upon the availability of highly active and cost-effective electrocatalysts. Current electrocatalysts are often constrained by challenging fabrication methods, including high temperatures, hazardous environments, and complex hydrothermal processes, which restrict scalability to an area of m² scale. In addition, the efficiency of water electrolysis hinges on the availability of highly active and cost-effective electrocatalysts. During operation in harsh conditions (e.g., extreme pH, high potential, and long-term service) for overall water splitting (OWS) electrolysis, electrocatalyst degradation (e.g., leaching) and poisoning are inevitable, potentially causing severe cross-contamination between electrodes with different components. Therefore, there is growing interest in designing and developing highly active, stable, and cost-effective bifunctional electrocatalysts capable of catalysing both HER and OER. Using the same materials for both reactions in a bifunctional catalyst is expected to address the issue of cross-contamination.

In my research, I developed NiFeCo catalysts for the oxygen evolution reaction (OER) using a solution-corrosion method. These catalysts demonstrate an ultralow overpotential of 149 mV at 10 mA/cm², are scalable to areas of 10 × 10 cm², and exhibit over 300 hours of operational stability in alkaline electrolyte.³ Furthermore, by incorporating trace amounts of iron into the NiFe(OH)_x OER catalysts, we created bifunctional NiFe(OH)_x/Fe/graphene catalysts also using the solution-corrosion method, to mitigate ingredient cross-contamination during overall water splitting achieving 10 mA/cm² under a cell voltage of 1.51 V.⁴ Additionally, I have developed multi-metallic bifunctional catalysts through electrodeposition method, which can be reproducibly fabricated on various substrates with a maximum area of 10 × 10 cm².⁵ These fabrication techniques are environmentally friendly and reproducible, holding significant potential for scalable hydrogen electrolyser applications in the future.

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The application of silicon anode materials in energy storage systems

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

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Ionic Transport in Solid or Semi-solid Materials for Electrochemical Energy Storage

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Abstract: To promote the application of next-generation battery active materials with higher specific and volumetric energies, various strategies have been employed to eliminate the associated challenges, such as volume change, poor ionic conductivity, unstable SEI layer, etc. In this talk, I will discuss our recent findings to address the issue of sluggish ion transport within the electrode bulk and electrode-electrolyte interface. I will also introduce our latest achievements in the understanding of the impact of the "lattice softening doping defect" on the kinetics of high-speed and stable cation diffusion, clarified the mechanism of competitive conduction of high-valence and low-valence cations in solid-phase materials, and achieved the goal of thermodynamic, kinetic, and stable regulation of charge carrier transport behavior at the electrode-electrolyte interface.

Regulation of Full Process of Photoexcited Charge Dynamics in Solar Fuels Production

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Photocatalysis relies on the activation of photoinduced charge carriers, which subsequently align themselves to facilitate targeted redox reactions. The behaviour of photoexcited hot carriers throughout the entire photo-mediated catalytic process plays a pivotal role in determining both the apparent quantum efficiency and the ultimate catalytic throughput. In this talk, the speaker will showcase recent research focused on controlling the comprehensive lifecycle of photoexcited carriers in solar driven catalytic chemical reactions, encompassing aspects such as excitation, separation, transportation, output, and thermalization. The goal is to enhance solar conversion efficiency for the sustainable production of clean fuels. The speaker will delve into the intricate relationship between functionality and performance, unveiling key design principles for optimizing photo-mediated catalysts. Furthermore, insights into reaction engineering will be shared, emphasizing strategies to maximize the yield of hot carriers for robust sunlight utilization and the generation of solar fuels.

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Triboelectric Nanogenerator-Powered Radio Frequency Identification Tags for Backscatter Communications

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Triboelectric nanogenerators (TENGs) were prepared through embedding synthesized perovskite barium zirconium titanate (BZT) core/metal silver shell nanoparticles into electrospun polyvinylidene fluoride-co-hexafluoropropylene (PVDF-HFP) nanofibers. The composite nanofiber mat based TENGs demonstrated more than 600% increase in output power compared to the neat polymer fiber mat. The top-performing TENG achieved an open-circuit voltage of 1339 V, a short-circuit current of 40 μA , and a power density of 47.9 W m^{-2} [1]. The Schottky junctions were built between the BZT nanoparticles and the smaller Ag nanoparticles distributed on their surfaces. These junctions enhanced charge carrier density in the tribo-layers, ensuring a high charge transfer rate while maintaining a low content of conductive fillers, thereby avoiding charge loss and improving performance. The high performance TENGs were integrated with radio frequency identification tags to enhance their maximum read range. The maximum reading range increased from 0.7 m to 3.4 m, which was a nearly five-fold enhancement. The additional sustainable energy source from TENGs presents a new approach to improve the usefulness of the backscatter communication tags, enabling the deployment of sustainable, autonomous and spectrally efficient 6G wireless networks.

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Leveraging dielectrophoresis at inertial flows for versatile manipulation of micro and nanoparticles

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The manipulation of micro and nanoparticles has extensive applications in biomedical research, clinical diagnostics, environmental monitoring, drug discovery, and the mining industry. Dielectrophoresis (DEP) uses non-uniform electric fields to manipulate particles, offering a label-free, high-precision, and non-invasive method compatible with various techniques for both natural and synthetic particles. While DEP manipulation has been well studied in the Stokes flow region with ultra-low Reynolds numbers ($Re \ll 1$), where fluid flow is dominated by viscous effects, its application in the inertial flow regime remains largely unexplored. This study aims to address the knowledge gap by coupling DEP and inertial flows for the manipulation of particles across micro and nano scales. First, we conducted a theoretical begin with a theoretical analysis of physical coupling of DEP and inertial lift forces along the vertical direction in microchannels, utilising symmetrical interdigitated electrodes (IDE) arrays patterned on the top and bottom channel surfaces. We then experimentally investigated how the vertical coupling of DEP and inertial lift forces affects particle lateral focusing properties. Finally, we demonstrated the applications of DEP in the inertial flow regime for size-based and dielectric property-based separation of particles and cells, as well as nanoparticle focusing and filtration. Leveraging DEP in inertial flows will advance the field by providing a versatile and powerful tool for the manipulation of micro and nanoparticles.

Enabling Controlled Polymer Structures for Advanced Applications

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The preparation of synthetic polymers with precise structures, compositions, and functions is a grand challenge in polymer science. Although synthetic polymers are often termed ‘monodisperse’, their primary structures are not as perfectly controlled as natural macromolecules, such as proteins and nucleic acid. The properties of the synthetic polymers result from the combination of individual molecules, each with unique performance. In this presentation, I will introduce a versatile and scalable strategy that is enabled by the combination of facile polymerization procedures (e.g., ATRP, RAFT) and ubiquitous purification processes (e.g., flash chromatography). This strategy is demonstrated to be applicable to a variety of polymer chemistries and structures on multigram scales with excellent mass recovery, and greatly simplifies the production of materials with increased control and homogeneity when compared to conventional strategies. At the end of the presentation, I will show several examples of using these well-defined polymers in high-value applications, including energy, wastewater remediation and theranostics.^[1-4]

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Biography



Dr Cheng Zhang is a Group Leader and an Australian Research Council DECRA Fellow (former National Health and Medical Research Council Fellow) at the Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland (UQ) where he leads a research group in polymer chemistry and PFAS remediation. His research focuses on the development of advanced polymerization, purification and characterization techniques to prepare well-defined functional polymers with precisely-tailored properties for important applications from PFAS remediation, energy materials e.g. solid electrolytes to functional biomaterials e.g. imaging and therapeutic agents. He has published over 85 journal articles, including *Nature Materials*, *Nature Reviews Materials*, *Chemical Reviews*, *Journal of the American Chemical Society*, *ACS Nano*, *Macromolecules* and etc. As CIA, he has successfully secured a number of competitive research grants from Australian Government, UQ and US DoD (>\$7 million AUD), regularly receives invitations to speak at national/international conferences (>30 to date), and has received numerous awards, including most recently Young Tall Poppy Award, Queensland Fresh Scientist, ACS Materials AU Rising Star, and UQ Industry Engagement Award.

Manipulation of strongly correlated electrons in monolayer 1T-NbSe₂

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Monolayer transition metal dichalcogenides can host exotic phenomena such as correlated insulating and charge-density-wave (CDW) phases. Such properties are strongly dependent on the precise atomic arrangements. In this work, we firstly provide experimental evidence of the quantum spin liquid (QSL) state in 1T-NbSe₂ via measurements of the Kondo effect in a 1T-1H heterostructure, further supported by measurements for magnetic molecules on 1T-NbSe₂ [1]. And then, we concentrate on the phase transition of correlated insulating states under 1D confinement [2]. We find out that the CDW phase of 1T-NbSe₂ can survive under both tensile and compressive strains. Moreover, significant strain-induced phase transitions are observed, i.e., tensile (compressive) strains can drive 1T-NbSe₂ from an intrinsic correlated insulator into a band insulator (metal). Furthermore, we find that the multiple electronic phases can coexist at the nanoscale [3].

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Enhanced Plant Stress Resilience through Quantitative Redox Regulation

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Adverse environmental factors, including extreme weather events (e.g. heat waves, droughts), soil salinity and pathogen attack, cause up to 70% of yield losses in major food crops. When plants are exposed to biotic and abiotic stress, the over-accumulation of “passive” (unwanted) reactive oxygen species (ROS) damages cellular components, resulting in phytotoxicity and growth inhibition. In contrast, under redox regulation, the production of “active” (desirable) ROS regulates redox signaling, activating defense pathways that foster plant acclimatization against stress. Enhancing the intrinsic ability of plants to survive and thrive under stressed conditions is thus critical to developing agricultural crops that are resilient to a changing climate. This can be achieved by quantitative redox regulation through quenching “passive” ROS to mitigate oxidative stress mediated by imbalanced ROS-ASC/GSH (ascorbic acid/glutathione) level as well as boosting “active” signaling ROS and thereby metabolically prepare the plant for further stresses, i.e., balanced redox state with concentrations of redox species in normal growth threshold. Through integrating NanoClay[1] for quantitative ROS scavenging and redox regulation with probe technology[2] for quantitative monitoring changes in the levels of redox species in situ in plants[3], recent studies in my group have developed Redox Responsive NanoClay for enhancing plant stress resilience through quantitative redox monitoring and regulation, which will be discussed in this talk.

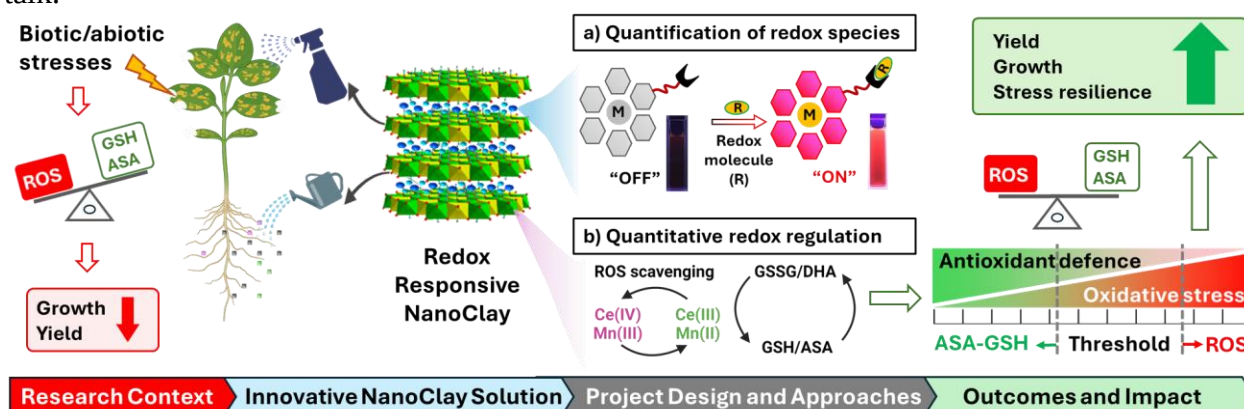


Figure 1. Schematic illustration of the development of “Redox Responsive NanoClay” to quantitatively monitor and regulate redox homeostasis for enhancing plants stress resilience.

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Infrared Reflection Absorption Spectroscopy Studies of the D₂O/Co(0001) Interface

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Studying thin ice structures at interfaces is a traditional yet highly active research field. In recent years, researchers have revealed the microscopic details of monolayer/bilayer thin ice structures by employing advanced surface science techniques such as scanning tunneling microscopy and atomic force microscopy. Techniques based on electron (such as scanning tunneling microscopy or photoemission spectroscopy) often encounter challenges related to conductivity when studying multilayer thin ice structures. Infrared reflection absorption spectroscopy (IRRAS) is another important technique for understanding thin ice structures.

In this study, we investigated the adsorption of water molecules on Co(0001) at 100 K using IRRAS and low-energy electron diffraction. For the first time, we experimentally revealed that D₂O adsorbed intact on Co(0001) surface forms hexamer islands with coexisting D-up and D-down geometries, in line with the “ice bilayer” model. Upon the completion of the first adlayer, a well-ordered ($\sqrt{3} \times \sqrt{3}$)R30° water layer structure emerges, featuring coexisting D-up and D-down domains in a ratio of approximately 2:3. This results in a surface with mixed hydrophilic and hydrophobic regions. As a second adlayer grows, water molecules preferentially adsorb on the D-up domain before distributing onto the D-down domain. The water adsorption on the D-down domains causes a reconstruction of the first water adlayer underneath, resulting in the transition from a well-ordered monolayer to disordered bilayers. Further increases in water coverage led to an amorphous ice structure.

Rational design of light-emitting materials in OLEDs

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Organic light-emitting diodes (OLEDs) are widely viewed as the basis for next generation displays and lighting. They are mainly organic materials without toxic metals such as mercury, and have fewer components and a thinner profile compared to lighting based on inorganic LEDs. However, to apply this technology widely and for it to reach its full potential, improvements in the emission efficiency and device lifetime are vital. So far, the development of blue, and especially deep blue, emitters in OLEDs has progressed rather slowly. Therefore, being able to predict the emission efficiency prior to the synthesis and measurement of properties is of crucial importance for the discovery of new highly efficient blue emitters.

Our work^[1-2] has shown that it is possible to predict the emission efficiency through the calculation of the radiative rate and non-radiative rate using state-of-the-art computational strategies. Specifically, we find that the main non-radiative process of a series of iridium(III) complexes is the elongation or even breaking of a metal-ligand bond, and the non-radiative rate (k_{nr}) can be predicted from the energy barrier to this non-emissive state.

In this talk, I will present our recent advances^[2] in quantitative calculation of the non-radiative rate of a family of iridium(III) complexes using approaches based on transition state theory and their application^[3] in proposing new highly efficient deep blue emitters for OLEDs.

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Numerical Study of Hydrogen Storage Design and Optimisation

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Efficient heat transfer is the key to hydrogen desorption in a metal hydride-based hydrogen storage system. In this study, a three-dimensional transient-state computational fluid dynamics (CFD) model is developed for describing the hydrogen desorption related heat/mass transfer phenomena inside a metal hydride-based hydrogen storage tank. The model involves flow, heat, and mass transfers related to hydrogen desorption in the storage tank. The model is validated against the temperature evolution data reported in the literature. The model is applied to a hydrogen storage tank where LaNi₅ is used as a metal hydride. The typical thermochemical phenomena related to the hydrogen desorption process are illustrated, including temperature evolution and hydrogen-to-metal-atomic ratio (H/M) during desorption. Further, several new tank designs are proposed and evaluated, including new heat management system configuration and phase change material application, for promoting heat transfer efficiency and hydrogen absorption/desorption performance. The simulation results indicate that the new design of embedding heating tubes, embedded copper fins, and aluminum foam additives shows the highest desorption performance in terms of both heating rate and hydrogen desorption rate, where the desorption rate is improved by 50% compared to the other designs. The employment of phase change material can make the metal hydride hydrogen storage tank operate as an independent system. This model is a cost-effective tool for designing, optimising, and scaling up hydrogen storage tanks.

Exploiting metal mobility in liquid metals for ammonia production

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The outlook for sustainable economic and ecological growth projects an ammonia economy as a key enabler to the energy transition landscape. Proponents of ammonia utilization, however, are subdued by the technical infeasibility and cost of advancing ammonia synthesis beyond the Haber-Bosch process [3]. Liquid metals are rapidly emerging as a new frontier in chemistry and have recently gained traction as an emerging class of catalysts that possess unique physicochemical properties [1,2].

This talk is primarily directed at the development of new catalytic materials for ammonia production by utilizing liquid metal colloids containing solid metal entities and intermetallic compounds. We utilize a liquid Cu-Ga alloy, capitalizing on the inherent atomic structure of the liquid metal, and the ability to modulate the electronic and geometric structures of liquid metal catalysts to drive the thermocatalytic synthesis of ammonia. The liquid metal alloy offers a dynamic metal complex with synergistic advantages that lift the activity of the individual metals, outperforming state-of-the-art ruthenium-based Haber-Bosch. Detailed analysis revealed that our new catalyst exploits a novel reaction pathway that is different from the conventional Haber-Bosch process, exhibiting high activity at low pressures. Gallium is found to activate the N-N bond, while the dissolved copper plays an important role in activating H₂, and ultimately releasing the gallium-bound nitrogen in the form of NH₃. The liquid state of the alloy also minimizes catalyst deactivation due to the highly mobile and self-refreshing surface of molten metals. This allows us to demonstrate high turnover numbers and excellent stability [4].

The developed approach facilitates exemplary alignment between high catalytic efficiency, robustness, and sustainable ammonia production that is predicated on the use of naturally abundant metals.

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ORAL PRESENTATION

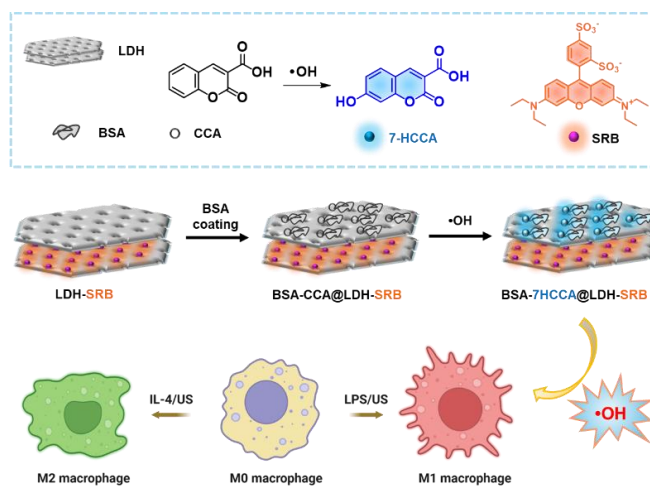
Responsive Nanoprobe for Ratiometric Fluorescence Detection of Hydroxyl Radical in Macrophage Polarization

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Quantification of hydroxyl radical ($\bullet\text{OH}$), one form of reactive oxygen species (ROS), plays critical roles in early diagnosis and treatment monitoring of various diseases. In this work, we report the development of a responsive nanoprobe for ratiometric fluorescence detection of $\bullet\text{OH}$ in macrophage polarization. The nanoprobe, BSA-CCA@LDH-SRB, was designed and prepared using coumarin 3-carboxylic acid (CCA) as the sensing unit for OH, and sulforhodamine B (SRB) loaded on layered double hydroxide (LDH) served as the fluorescent reference component. The coupling of CCA to bovine serum albumin (BSA) and the loading of BSA-CCA on the surface of LDH enabled the nanoprobe for fluorescence detection of $\bullet\text{OH}$ with high sensitivity and minimal interference from other biomolecules, ions, and ROS. The emission of the prepared BSA-CCA@LDH-SRB at 444 nm emerged and the intensity was increased according to the concentration of $\bullet\text{OH}$, while the emission at 580 nm was maintained, allowing the nanoprobe for ratiometric fluorescence ($F_{444/580}$) detection of $\bullet\text{OH}$. Loading of the BSA protein on LDH surface, the biocompatibility and colloidal stability of the LDH-based fluorescent nanoprobe were further improved, facilitating the detection of $\bullet\text{OH}$ generation in macrophage polarization stimulated by biomolecules and physical ultrasound irradiation. This study thus offers a new nanoprobe as the tool for investigating $\bullet\text{OH}$ evolutions, advancing the biomedical investigations of macrophage polarization associated inflammation.



Scheme 1. The schematic design of the nanoprobe (BSA-CCA@LDH-SRB) for $\bullet\text{OH}$ detection in macrophage polarization activated by lipopolysaccharide (LPS), interleukin-4 (IL-4) and ultrasound treatment.

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Gas-Phase Fluorination of Boron Nitride Nanotubes

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Boron nitride nanotubes (BNNTs) possess unique chemical, physical, thermal, and electrical properties which have made BNNTs a promising type of material for applications, such as in fabricating micro and nanoelectromechanical devices [1],[2],[3],[4]. Theoretical and experimental studies have shown the possibility of obtaining new BN- or BNNT-based materials through surface functionalization, which could possess interesting electrical and magnetic properties compared to pristine h-BN and BNNTs [5],[6],[7]. In this talk, I will discuss the fluorination of BNNTs using molecular F₂, with a focus on controlling the degree of fluorination by adjusting the fluorination conditions, including temperature and the ratio of gas mixtures. I will present the results from a range of characterizations of the fluorinated BNNTs to demonstrate the structural and morphological transformations after fluorination and to understand the reaction mechanism and the nature of the bonding between fluorine with boron and nitrogen atoms.

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Development and Applications of Radioisotope Thermoelectric Generators (RTG)

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Radioisotope Thermoelectric Generators (RTG) utilize nuclear decay heat from radioactive isotopes to generate electric power, without employing moving parts. RTGs can work unattended for decades with a relatively steady power output, making them ideal power sources for deep space explorations. [1] Among many space power systems, RTGs have consistently demonstrated unique capabilities. Photovoltaics is indeed a mature power technology for earth-orbit missions, where sufficient solar power is available. However, RTGs become irreplaceable when it is impossible to collect solar energy. For example, exploring shadowed areas on planetary surfaces and deep space which is too far away from the sun. RTGs have demonstrated long serving life and reliable operation with compact design in radioactive and other extreme environments through their service history in space. Therefore, RTGs are ideally suited for deep space missions with complex environmental conditions where solar energy is impractical. [2]

The Plutonium-238 (Pu-238) has so far been the most used isotope fuel for RTGs in space applications, due to its long half-life of 87.7 years, high thermal power density of ~0.56 watts per gram, and alpha emission which is easy to shield. However, fabrication of Pu-238 is extremely complicated and expensive, making it desirable to develop new radio isotope fuels as replacement. Besides fuels, thermoelectric materials, which can generate electric power via temperature gradient, are the key component of the heat-to-electricity convertor. [3] So far PbTe and SiGe-based thermoelectric materials have been successfully used in RTGs, providing electric power for spacecrafts from dozens of to hundreds of watts electric (We). However, the efficiency of the current RTGs is at a low level (< 10%) compared to other electricity generation systems such as chemical and solar batteries. Therefore, there's a lot of room for improvement by incorporating novel thermoelectric materials with high performance, carefully designing the architecture of the RTG. [4]

The development and application history of RTGs will be comprehensively introduced in this presentation, following by an outlook on the state-of-the-art high performance thermoelectric materials and concepts of RTG design.

Keywords: Radioisotope Thermoelectric Generator (RTG), Thermoelectric Materials, Thermoelectric Devices

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ABSTRACTS

Synthesis and catalytic properties of metal nanomaterials with unconventional crystal phases

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Metal nanomaterials have excellent intrinsic catalytic activity, high electrical conductivity and high stability, making them promising catalyst materials. However, conventional colloidal synthesis mainly focuses on the morphology and composition control of nanocrystals. This talk will introduce some interesting discoveries we have recently made in the aspect of crystal phase control of metal-based nanocatalysts and their enhanced catalytic performances. For example, traditional Au nanomaterials have the same face-centered cubic (*fcc*) crystal structure as bulk gold, while we have developed unconventional 4H/*fcc* heterogeneous Au nanorods with high yield. Au nanorods in these unconventional crystal phases have high thermal stability and can serve as high-quality seeds for epitaxial growth. Therefore, we further prepared unconventional 4H/*fcc* core-shell nanostructures, in which Au was coated with other catalytically active metals (such as Pd and Cu). The catalytic performances of these new crystal phase metal nanomaterials in ethanol electrooxidation, and carbon dioxide electroreduction were studied. In a latest work, we used Pd-based nanocrystals of different crystal phases as seeds, further deposited Pt surfaces of different crystal phases by colloidal epitaxial growth, and carried out phase-dependent performance analysis of Pt surfaces in heterogeneous selective hydrogenation reaction. The Pt surfaces with unconventional crystal structures show better selectivity and durability compared to conventional *fcc* Pt. These works demonstrate a new strategy to design and synthesize the crystal phase of metal nanomaterials by wet-chemical method, and explore the effect of crystal phase regulation on various properties of metal nanomaterials.

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

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Power-to-gas (P2G) processes, by converting electricity from renewable energy to H₂ and then into other high value-added and energy-intensive chemicals, such as methane in the presence of active catalysts, have become an effective solution via CO₂ reduction pathway [1]. Production of methane through CO₂ methanation/Sabatier reaction is an exothermic reaction ($\Delta G_{298K} = 130.8$ kJ/mol) where H₂ and CO₂ form CH₄ and H₂O. Novel catalysts for CO₂ hydrogenation to CH₄ still need to be developed to reach high activity at low temperatures, high selectivity in desired products, and resistance to sintering and coke formation [2]. It is affected by many other factors, such as the support phase, metal loading, catalyst preparation, pre-treatment, and testing conditions. Metal/oxide (M/O) composites are the most widely used multi-component supported catalyst systems. M-O interfaces have been demonstrated to be important in determining their catalytic performances^{1,2}. Engineering and understanding the M-O interface are thus essential to guiding and designing catalysts for excellent catalytic performance.

In this study, we are investigating CO₂ methanation over Ru as metal and ZrO₂ as support. Preliminary catalytic screening on 5 wt % Ru/ZrO₂ catalyst showed that reduction pre-treatment at 600 °C showed a high conversion of CO₂ and exhibited a high selectivity towards CH₄ (>98 %). CO₂ conversion reached a maximum (~85 %) at 300 °C, and a further increase in reaction temperature decreased CO₂ conversion. This could be a combined effect of the decomposition of methane to CO/CO₂ and the water gas shift reaction of CO to CO₂. The pre-treatment reduction at 600 °C generated variable oxidation states of Ru, i.e. Ru⁰, Ru³⁺ and Ru⁴⁺. A further mechanistic study of CO₂ methanation over Ru/ZrO₂ catalyst by *In situ* FTIR and DRFITS studies showed that methane production occurs through formate/carboxylate surface intermediates – formed by the reaction of (bi)carbonate with H_{ads} spillover from metallic Ru [3, 4].

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Development of Carbon Fibre Electrodes for “Massless” Energy Storage via Surface Modification Approaches

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In the pursuit of multifunctional and lightweight materials, carbon fiber-reinforced composites (CFRCs) have emerged as versatile solutions with significant environmental and economic benefits. This study introduces innovative surface modification strategies to enhance CFRCs for energy storage applications while contributing to sustainability efforts.

For supercapacitors, redox-active poly(o-phenylenediamine) (PoPD) is covalently grafted onto unsized T300 carbon fibers via electro-initiated polymerization, followed by $\text{Ti}_3\text{C}_2\text{T}_x$ MXene dip-coating. This hybrid coating improves the interfacial shear strength of CF by 54% while maintaining tensile properties. Electrochemically, the capacitance of CF increases to 157 F g^{-1} , a remarkable ~ 725 -fold enhancement over pristine CF, with the MXene coating providing superior electromagnetic interference (EMI) shielding. A structural supercapacitor device fabricated with PoPD-MXene coated CF electrodes, glass fiber separators, and an epoxy-solvate ionic liquid solid electrolyte achieves a capacitance of 908 mF g^{-1} , 99% coulombic efficiency, and 94% capacitance retention over 5000 cycles.¹

For Zn batteries, CF is functionalized for both anodes and cathodes, enabling the development of an all-carbon fiber composite Zn battery with bicontinuous solid polymer electrolytes. The surface modification strategies employed in this study were optimized to graft $\alpha\text{-MnO}_2$ onto carbon fiber and to facilitate the electroplating of Zn. The interfacial adhesion between the carbon fiber and the deposited layers was enhanced through pretreatment with diazonium salts, which improved the chemical compatibility and bonding at the interface. This approach ensures a robust and stable attachment of active materials, critical for the performance and longevity of energy storage systems.

The solid polymer electrolytes used in these studies are recyclable, offering significant sustainability advantages², and the surface modification approaches are highly translatable to existing CF production lines, further reinforcing its viability for large-scale applications.

This work not only highlights the potential of modified CFRCs in structural energy storage and EMI shielding but also underscores their role in promoting sustainable materials solutions for aerospace, automotive, and defense industries.^{3, 4}

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Theoretical Screening of P-block Single Atom Anchored on g-C₃N₄ for NO Reduction to NH₃

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Ammonia (NH₃) has been seen as a highly value-added energy storage medium and plays an important role in the agricultural and chemical industries. Industrial production of ammonia (Haber-Bosch Process) requires harsh reaction conditions (specific pH, high temperature and pressure), leading to huge energy consumption and CO₂ emissions. The inertness of non-polarizable N₂ with high dissociation energy (941 KJ/mol) limits the Faradaic Efficiency (FE), making it impractical to mass-produce the ammonia. Alternatively, nitric oxide (NO) is the promising nitrogen source with a relatively low bond energy of 630.57 KJ/mol as well as high solubility. Thus, the electrochemical reduction of nitric oxide to ammonia is a practical solution for closing the nitrogen cycle and generating valuable chemical products.

Recently, two-dimensional (2D) materials have been widely used in the electrocatalytic field due to their vast surface, high conductivity and abundant active sites, whose performance can be improved through atom doping, defect creation or surface engineering. Graphitic carbon nitride (g-C₃N₄) is a 2D metal-free photocatalyst with a visible light response and tunable electronic structure. The N-surrounding vacancy can also accommodate the single atoms (SACs) for the application in many reactions such as HER, NRR and CO₂RR. Apart from the usage of transition metal-based catalysts, the p-block elements also exhibit high performance as reported by many works. Herein, it is intriguing to develop p-block single-atom catalysts for the electroreduction of NO to NH₃.

In this presentation, we will demonstrate the catalytic potential of p-block SAC@g-C₃N₄ for NORR process. The screening criteria are proposed in terms of stability, selectivity and activity. The stable anchoring of SACs on the substrate is examined. The favourable NO adsorption over proton is also compared with the limited performance of hydrogen evolution reaction (HER). The minimum free energy change is plotted with thermodynamically favourable intermediates and the promising B-based catalyst with a low limiting potential of -0.02 V is screened. The origin of high activity is due to the p orbital matching and charge transfer between B@g-C₃N₄ and NO. Overall, our work screened the promising metal-free SAC catalysts for the NORR process and highlighted the important role of p-block elements in electrocatalytic applications.

Anomalous Ion Transport Properties Induced by Ion Pairing and Ion Clustering inside Sub-1nm Graphene Nanoslits

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The intriguing phenomena of ion pairing and salt aggregation inside two-dimensional nanoslits have recently been reported in experiments and numerical simulations, leading to anomalous ion transport phenomena, such as the gate-voltage modulated ion diffusion and the memo-resistive properties [1,2]. However, there are still many challenges to understand the physical origins and to explore new opportunities. On the one hand, observing ion transport behaviours at the atomic level is challenging due to technological constraints. On the other hand, theoretical studies often rely on mean-field approaches that are inadequate for accurately capturing cation-anion correlations [3,4]. Consequently, the atomic-level mechanisms associated with the correlated transport of ion pairs and clusters remain elusive.

In this study, we utilize Molecular Dynamics (MD) simulations to explore the effects of ion pairing and clustering on both ion diffusion and ion migration within sub-1nm graphene nanoslits. Employing a novel analytical method [5], we accurately measure the contribution of each cluster to these ion dynamic properties, and uncover several interesting discoveries. First, under nanoconfinement, ion clusters maintain faster diffusion rates than traditionally expected, as the decrease in their diffusion coefficient with increasing size occurs more slowly than predicted for bulk solutions. Secondly, by applying an adjustable in-plane electric field, the size, lifetime, and transport directions of these clusters can be modulated. In this way, we first report the negative differential conductance (NDC) for sub-1nm nanoconfined electrolytes, *i.e.*, at low electric field strengths, the ionic conductivity will first decrease with the increased E-fields. This behaviour opens new possibilities for developing components in ionic circuits, such as oscillators, amplifiers, and logic gates. Finally, both anions and cations show a wide range of controllable transfer number under low electric field strengths (e.g., from -1.82 to $+1.74$ for Na^+ ion under $0.02 \text{ V/\AA}$ to $0.04 \text{ V/\AA}$ E-fields), which introduces novel design principles for nanoconfined electrolytes.

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Oxygen Driven Defect Engineering of Monolayer MoS₂ for Tunable Electronic, Optoelectronic, and Electrochemical Devices

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Background and Aim

Two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) are emerging as suitable alternative semiconducting material to the existing silicon-based electronics and optical technologies. The performance of TMDs such as monolayer MoS₂ relies on the quality of 2D atomic crystals, which can be influenced by atomic defects such as sulfur vacancies (V_s) and atomic substitutions [1,2]. Achieving reliable and scalable defect engineering in monolayer MoS₂ poses significant challenges. Usually requiring a two-step process that includes aggressive post-synthesis processing with detrimental effects on monolayer MoS₂. This work demonstrates a simple, effective, and scalable strategy to inherently regulate the formation and/or the passivation of V_s defects on demand within monolayer MoS₂, by tuning the pressure during chemical vapour deposition (CVD) growth [3].

Methods

CVD was used to obtain monolayer MoS₂ crystals in low pressure (LP) oxygen deficient and atmospheric pressure (AP) oxygen rich conditions [3]. Standard photolithography techniques were deployed for devising two terminal lateral devices [3].

Results

LP CVD-grown MoS₂(LP-MoS₂) had V_s induced defect-rich crystals primarily attributed to the oxygen-deficient growth conditions. Conversely, AP CVD-grown MoS₂(AP-MoS₂) passivates these defects with oxygen from ambient conditions [3]. This disparity in defect profiles profoundly impacts functional properties and device performance. The n-doping induced in LP-MoS₂ generates enhanced photoresponsivity and detectivity in fabricated photodetectors compared to the AP-MoS₂-based devices [3]. Defect-rich LP-MoS₂ outperforms AP-MoS₂ as channel layers of field-effect transistors (FETs), as well as electrocatalytic material for hydrogen evolution reaction (HER) [3].

Conclusion

We have demonstrated the effectiveness of our in-situ defect engineering strategy for customizing TMDs such as MoS₂, for targeted applications in optoelectronics, electronics, and catalytic devices.

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Tailoring the multifunctional properties of self-assembled cellulose nanocrystal (CNC) photonic films for advanced applications

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Structural color is prominent in several biological entities such as bird feathers, insects, plants, and aquatic creatures where the color is originated from the self-assembly of biological building blocks, such as protein, chitin, and cellulose at nanoscale. Of these, cellulose is the highly abundant as well as inexpensive biological building block. In recent years, the research on the controlled production of structurally colored cellulose nanocrystal (CNC) films has received increasing interests for different applications, including optical coatings, mechanical sensors, soft displays, anti-counterfeiting materials, information encryption, cosmetics and many more. However, significant challenges remain in the production and application of CNC-based structural color such as inherited brittleness, low thermal stability, static optical properties, highly hygroscopic nature, longer evaporation times. This research addresses these limitations by developing advanced CNC-based photonic polymer composites with enhanced thermal stability, reduced hygroscopicity, maintained optical properties, and improved mechanical performance using biobased additives. The resulting CNC-photonic polymer composites are explored for the applications in colorimetric sensors and anticounterfeiting materials. This study not only contributes to the fundamental understanding of chiral nematic nanocellulose-based composites but also opens avenues for innovative and sustainable solutions in the diverse technological aspects such as advanced coatings, security labels, radiative coolers, and smart sensors.

Keywords: cellulose nanocrystals, chiral nematic, photonic materials, biobased additives, sensors.

Balancing Polysulfide Containment and Energy Loss in Lithium-Sulfur Batteries

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For Lithium–sulfur batteries, Microporous membranes have been widely investigated as a potential solution strategy to ‘polysulfide shuttle effect’. However, an often-overseen consequence of this strategy is the unintended hindrance to lithium-ion mobility, which compromises the battery energy density (Figure 1). This study sheds light on these effects, using Li–S batteries as a representative model, by assessing the challenges of lithium-ion transport through a range of micro- and meso-porous membranes.

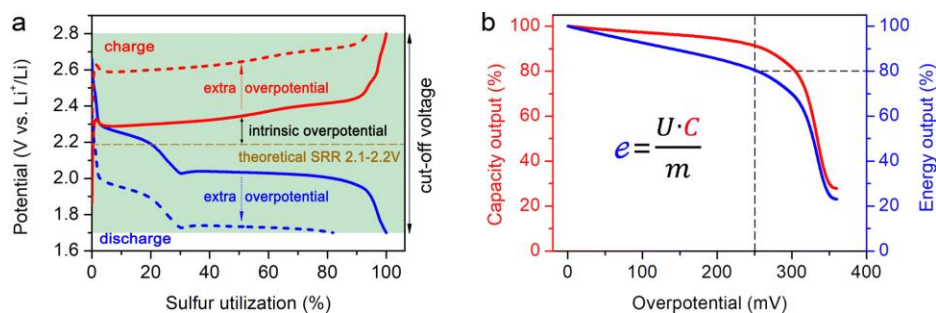


Figure 1 Correlation between overpotential and energy density loss in a model Li-S coin cell¹

In this research, we investigated the energy losses induced by seven membrane candidates for Li–S batteries. Our experimental findings indicate that Li–S batteries using a commercial PP separator undergo a minimum energy density reduction of 20% when overpotentials exceed 250 mV. The introduction of a microporous membrane as polysulfide barrier onto the PP separator significantly increases energy loss. Li|Li symmetric cell tests demonstrate that certain types of membranes (including GO, MoS₂, and rGO) display overpotentials surpassing 250 mV at 1C rate. This issue becomes more pronounced when these membranes are tested within H-cells. Fabrication and testing of porous membrane with an induced level of mesoporosity (e.g., holey graphene membranes) and modeling confirm that the overpotentials stem from physical obstruction of Li⁺ transport, revealing the need to compromise between soluble polysulfide blocking and energy loss. For constructing efficient batteries, the optimal effective hole area percentage should be close to commercial PP separators (~15.5%), i.e., small enough to mitigate the species shuttle effect and to prevent internal short circuiting but large enough to avoid detrimental increments in overpotential. Holey graphene membranes with 13.5% and 9.1% of surface holes can decrease the polysulfide diffusion by 62.5% and 113%, while increasing the overpotential for Li⁺ transport by only 33.3% and 60%, respectively. These insights chart a path for the design of multi-scale porous membranes for emerging rechargeable batteries.

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Water-Based Recovery of FTO/SnO₂ Substrate for Sustainable Perovskite Solar Cell Technology

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Proper recycling strategies are critical in reducing waste while mitigating the environmental impact of toxic materials. As a rapidly emerging technology the re-use of valuable material components for end-of-life perovskite solar cells (PSCs) should be planned in a sustainable way. The fluorine-doped tin oxide (FTO) substrate is an important and expensive component in PSCs, which accounts up to 40% of a typical PSC raw material cost. In this study, we investigated the effect that a series of solvents including dimethylformamide (DMF), dimethyl sulfoxide (DMSO), Acetone, hot (80 °C) water, and Acetone/water mixture has on the properties of the substrate recovered from the PSCs after a solvent washing process.

The results show the influence on both the surface wettability and electronic properties of SnO₂/FTO after a solvent-washing recycling process. Specifically, the surface wettability of SnO₂/FTO is largely unchanged with water washing while a dramatic increase of surface hydrophobicity is obtained when an organic solvent is used. Among the solvents, acetone had the most undesirable effect on recycling. Washing with acetone led to the largest increase in surface water contact angle, caused a significant upward energy level shifting of the conductive band by 150 meV. This resulted in the SnO₂/FTO recovered using acetone washing, having an obstructive energy barrier for interfacial charge injection from the adjacent perovskite film. In contrast, water-based recycled substrates resulted in a slight downward energy level shift of the conduction band (180 meV), creating more favorable interfacial charge injection as confirmed by photoluminescence experiments. As a result, PSCs using a water-based recycled SnO₂/FTO substrate produced a high-power conversion efficiency (PCE) of 19.33% which is much higher than that achieved with organic solvent washing and is promisingly comparable to that of a fresh unused SnO₂/FTO substrate (PCE = 19.85%) [1]. Furthermore, we demonstrated that water washing can maintain the SnO₂/FTO substrate in an excellent condition and retain comparable PSC performance for up to four re-use cycles. This simple water wash method is the most effective method of recycling SnO₂/FTO compared with organic solvent washing methods. It will ultimately accelerate the PSC transition to sustainable commercialization.

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Spatial Porosity Patterning in 4D Hydrogels via Dynamic Interface Printing of Aqueous Two-Phase Emulsions

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Within the biomedical field, strategies for tailoring the mechanical and microstructural properties of 3D cell culture scaffolds are highly sought after for applications in tissue engineering and in vitro disease modeling[1]. To this end, aqueous two phase emulsions have attracted much attention in recent years because of their relative convenience in biological systems and the range of biocompatible materials that can be used to create them[2]. By controlling the solution conditions, previous work has demonstrated the ability to form pore networks of varying size and connectivity inside hydrogels[3]. However, the parameters that are often controlled (temperature, pH, pressure, component functionalization) limit researchers' ability to encapsulate cells within the hydrogel material during fabrication; incompatible solution conditions necessitate that cells are seeded into or onto the scaffold afterwards, introducing additional complications and potential failure points. Additionally, although 3D bioprinting methods have been used to create microporous hydrogels based off two-phase emulsions, the structures created possess only a uniform porosity throughout their bulk[4]. Using our novel biofabrication technique, Dynamic Interface Printing[5], we have demonstrated our ability to control the separation of gelatin methacrylate/polyvinyl alcohol (GelMA/PVA)-based aqueous two-phase emulsions and thus the pore size of hydrogels created from photocuring those emulsions. Preliminary studies have shown a range of achievable pore sizes of 6 to 80µm. This enables us to spatially pattern porosity in 3D cell culture scaffolds using a combination of acoustic- and light-based patterning. This tunable porosity can also be used to tailor the mechanical properties of the resultant hydrogels, both in terms of its bulk and its microstructure. Our technique has been shown to reliably induce spinodal decomposition of the emulsion, meaning that the pores created within the resulting hydrogels are consistent in size and well interconnected. By leveraging dityrosine-based crosslinking to cure the polymer blend, we can control the dissolution rate of the porogen phase, enabling strategies for 4D cell culture in the future[6]. We show that our method can create consistent pore sizes and interconnectivity throughout the bulk of the fabricated constructs, thereby demonstrating its utility for a wide range of biomaterial-based applications. In particular, the ability to create a range of pore sizes within fabricated constructs without the need to change material or dynamically adjust solution conditions during fabrication represents a significant advantage to researchers hoping to studying cell-material interactions for regenerative medicine purposes.

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From Waste to Value: High-Quality Precipitated Silica from Rice Hulls for Green Manufacturing

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Precipitated silica is a critical nanoadditive widely used in industries such as rubber, plastics, and coatings, with growing market demand due to its applications in improving durability, energy efficiency, and product performance [1]. However, traditional methods of producing precipitated silica from quartz sand are energy-intensive and environmentally harmful. This has driven the search for more sustainable alternatives, with silica-containing agricultural wastes like rice hull emerging as a promising feedstock [2].

We developed an innovative process for converting rice hulls and rice hull ash (RHA) into high-quality precipitated silica in laboratory and pilot scales. Our processes not only offer a sustainable alternative to the quartz-based method but also help in managing agricultural waste. The protocol we developed allows precise control over the size, morphology, and shape of silica particles, enabling their customization for various industrial applications. Comprehensive characterization of the precipitated silica was carried out using techniques such as BET surface area analysis and XRD, demonstrating that our methods produce high-purity, amorphous silica with properties comparable to or surpassing those derived from conventional sources.

The precipitated silica was subsequently used as a filler in rubber composites, where it demonstrated comparable performance to commercial precipitated silica in terms of mechanical properties and reinforcement behavior. A technoeconomic analysis was also conducted, revealing the cost-effectiveness of the process, with a reduction in production costs and a lower environmental impact compared to conventional methods. These findings position rice hull-derived silica as a competitive and sustainable alternative in the growing market for silica-based materials.

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Large-Area Transfer of Nanometre-thin C₆₀ Films

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Fullerenes, with well-defined molecular structures and high scalability, hold promise as fundamental building blocks for creating novel carbon materials.^{1–3} The fabrication and transfer of large-area films with precisely controlled thicknesses and morphologies on desired surfaces are crucial for designing and developing new fullerene-based materials and devices.^{4,5} In this talk, I will present strategies for solid-state transferring C₆₀ molecular nanometre-thin films, with dimensions of centimetres in lateral size and thicknesses controlled in the range of 1–20 nm, onto various substrates. Furthermore, I will discuss the preparation of centimetre-wide graphene/C₆₀/graphene heterostructures through layer-by-layer stacking of C₆₀ and CVD-grown graphene films. This transfer methodology is versatile, allowing for the complete transfer of chemically modified C₆₀ films, including oxygenated C₆₀ films and C₆₀Pd_n organometallic polymer films. Additionally, direct solid-state transfer of C₆₀ and C₆₀Pd_n films onto electrode surfaces has enabled their electrocatalytic performance for the hydrogen evolution reaction to be probed directly. This thin-film transfer strategy⁶ facilitates the facile preparation and transfer of large-area C₆₀ films, offering a distinct platform for fullerene chemistry and experimental synthesis of novel carbon structures.

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Screening Furfural-Copper Adsorbate-Surface Geometries using low-cost Computational Methods

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Furfural derived from lignocellulosic biomass is a platform chemical which serves as a basic building block for various chemical industries. Valorised from the hydrolysis and dehydration of hemicellulose, it is used for the catalytic conversion to furfuryl alcohol and diols, essential to the synthesis of resins, lysine, vitamin C and other C4 and C5 chemicals downstream. Hence, developing efficient heterogeneous catalysts is central to improving the downstream utilisation of furfural. [1-3]

Previous studies of structure-function relationships of heterogeneous catalysts indicated that their reactivity is not confined to a single well-defined active site. Instead, numerous sites contribute to a catalyst's performance, with multiple reaction pathways and hundreds of elementary steps occurring simultaneously. Therefore, improving the efficiency of heterogeneous catalysts and their reaction conditions requires fundamental insights into each active site, systematically probing different adsorption geometries and positions. [4]

Density functional theory (DFT) methods are essential for accurately modeling such catalytic systems. However, their computational demand increases significantly with the molecular size of the adsorbate, creating a bottleneck when screening possible adsorption conformations. To mitigate this, machine learning-assisted methods, particularly machine-learned interatomic potentials (MLIPs), and multi-level modeling approaches utilizing low-cost semi-empirical quantum-chemical methods (SQMs) have shown great potential. [4, 5]

Here, we present a multi-level modelling approach combining low-cost computational methods with DFT to relax the geometries of randomly positioned furfural on different flat and edged Cu-facets, screening for low-energy ensembles of adsorption configurations.

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Optimisation of additives to maximise performance of expandable graphite based intumescent flame-retardant polyurethane composites

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The importance of the work is to address a critical need for a country (Australia) prone to bushfires, which is new trajectories for fire-resistant materials and their fabrication. Polyurethane (PU) and other foams are used widely in padding for furniture, vehicles, and construction elements. However, these foams are very flammable, so there is widespread research that seeks new way to minimise the risk of fire with this material. This research work on the development of sustainable and composite materials for advanced manufacturing products.

The effect of varying the weight percentage composition (wt.%) of low-cost expandable graphite (EG), ammonium polyphosphate (APP), fibre glass (FG) and vermiculite (VMT) in Polyurethane (PU) polymer was studied using a traditional intumescent flame retardant (IFR) system. The synergistic effect between EG, APP, FG and VMT on the flame-retardant properties of the PU composites was investigated using scanning electron microscope (SEM), thermal gravimetric analysis (TGA), tensile strength tests, and cone calorimetry. The IFR that contained PU composites with 40 wt.% EG displayed superior flame-retardant performance compared with the composites containing only 20 wt.% or 10 wt.% EG. The peak heat release rate, total smoke release and carbon dioxide production from the 40wt.% EG sample along with APP, FG and VMT in the PU composite was 88%, 93% and 92 % less than the PU control sample, respectively. As a result, the synergistic effect was greatly influenced by the compactness of the united protective layer. The PU composite suppressed smoke emission and inhibited air penetrating the composite, thus reducing reactions with the gas volatiles of the material. SEM images and TGA results provided positive evidence for the combustion tests. Further, the mechanical properties of PU composites were also investigated. As expected, compared with control PU, the addition of flame-retardant additives decreased tensile strength, but this was ameliorated with the addition of FG. These new PU composite materials provide a promising strategy for producing polymer composites with flame retardation and smoke suppression for construction materials.

Controllable Cu nanofoam with spatial confinement for enhanced C₂ selectivity in CO₂ reduction

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Nanowire catalysts have been extensively used in energy conversion, including CO₂ reduction reactions (CO₂RR), due to their favorable surface areas and active sites. However, the impact of bending nanowires on local micro-environment tailoring and CO₂RR selectivity remains unclear. This study investigates the tunability of spatial confinement by partially bending Cu nanowires to form nanofoam and its effect on CO₂RR selectivity. Cu nanofoams were synthesized through wire-length-guided bending of the Cu(OH)₂ nanowires, followed by electrochemical reduction to Cu nanowires. This facile synthesis method allowed for the controlled production of Cu nanofoam electrodes with varying densities. We demonstrate that the selectivity for C-C coupling in CO₂ hydrogenation to form ethylene-dominated C₂ products at a fixed potential can be tuned by systematically altering the Cu nanofoam density. The local confinement tailoring capacity on CO₂RR is primarily influenced by enhancing the mass transport, adjusting micro-environment and tuning local pH within the Cu nanofoam, which promote the formation of C₂ products through a preferred hydrogenated C-C coupling pathway. This study highlights the potential of Cu nanofoam electrodes in tuning hydrocarbon selectivity via simple control of nanofoam density, offering valuable insights into designing efficient catalysts for converting CO₂ into multi-carbon products.

Surface reconstructions in nitrate reduction reaction for electrocatalytic ammonia production

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The electrochemical nitrate reduction (e-NO₃RR) is considered as one of the most promising candidates for green ammonia synthesis due to the high solubility of NO₃⁻ in aqueous solutions, and its widespread presence in agricultural and industrial wastewater. The cobalt-based catalysts have been widely studied for ammonia production by e-NO₃RR. However, the unavoidable reconstruction of these catalysts under reduction potentials was seldom discussed in previous works. It is essential to deeply understand the reconstruction mechanism for realizing efficient ammonia production by controlling the well-designed reconstructed nanostructures. In our work, the Co-based materials attain efficient nitrate reduction and selective ammonia production, which is superior to the benchmark catalysts. Meanwhile, the reconstruction mechanism of Co₃O₄ during e-NO₃RR process is systematically studied by investigating the influences of incorporation elements and applied potentials. Moreover, the potential-determined mechanisms of different Co-based materials were revealed by the combination of experiments and calculations. These studies may shed new light on the design of highly efficient electrocatalysts for enhanced ammonia production.

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Heterogeneous Biocatalysis Cascade Systems and Cofactor Recycling

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Cofactor-dependent biocatalysis systems exhibit significant value and extensive application potential in the broad fields of organic synthesis due to their substantial and diverse enzyme species and catalysis reaction types. However, native enzymes and cofactors inherently have drawbacks of high cost, poor stability, and difficulty in recyclability, which greatly hinder the large-scale applications of biocatalysis systems in practical processes. To address the above issues, this research topic therefore focuses on constructing efficient, robust, and cofactor-recyclable heterogeneous biocatalysis cascade systems through establishing cofactor regeneration systems and utilizing immobilization technology.

First, nicotinamide cofactor (NAD)-dependent alcohol dehydrogenase (ADH) and amine dehydrogenase (AmDH) were site-specifically co-immobilized onto silica nanoparticles (SNPs) by using a silica-binding peptide (SiBP) for biosynthesis of chiral amines [1]. Compared with the corresponding free system, the chiral amine yield with the prepared co-immobilization system increased 85%. Second, based on the above research work, both the negative-charged reduced nicotinamide cofactor (NADH) and the SNPs-bound dual-enzyme (ADH-AmDH@SNPs) were co-encapsulated into the positive-charged microgel (PVCL-Vim) through electrostatic interactions and gel swelling, thus leading to the efficient cascade reaction and outstanding cofactor recycling [2]. The PVCL-Vim microgel could not only electrostatically adsorb NAD but also provide the cofactor molecules with high mobility, which guaranteed accessibility of the immobilized NAD to the enzymes. Third, a novel strategy for co-encapsulating NADH, ADH, and AmDH within a hydrogen-bonded organic framework (HOF) through the assistance of polyelectrolyte was developed [3]. The polyelectrolyte played two key roles: as a carrier for electrostatically binding NADH and as a protective coating for enzymes against the adverse interactions of HOF monomers. Thus, this strategy also addressed the prevailing issue of the compromised activity recovery associated with biocatalysts embedded in HOFs. In addition, this co-immobilization approach was successfully applied to the co-encapsulation of the cascade system involving nicotinamide phosphate cofactor (NADP)-dependent phenylacetone monooxygenase (PAMO) and phosphite dehydrogenase (PTDH). Both the constructed co-immobilization systems of the cofactor-dependent multienzyme cascades exhibited boosted cascade performance and stability.

This research presents the design and implementation of novel co-immobilization systems for cascade biocatalysis and cofactor recycling, utilizing four oxidoreductases and two cofactors. The efforts and success opened a new avenue for the application of oxidoreductase cascade biocatalysis in the synthesis of high-value chemicals.

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Regulating ion migration maximizes electricity generation from ambient moisture

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Harvesting energy from moisture has emerged as a promising solution to meet future demands for low-carbon energy [1]. However, the low and intermittent electrical output of moisture-electric generator (MEG) significantly limits its practical applications. Herein, we designed and fabricated a novel device using magnetron sputtering to deposit a metal electrode onto a high-porosity substrate and through the optimisation of the internal ion migration to enhance power generation from ambient humidity. When exposed to ambient humidity, this uniquely designed system generates an open-circuit voltage exceeding 1.5 V and a current density over 1.2 mA cm⁻², both sustained for more than 200 h. The enhanced electrical output and stability is primarily attributed to accelerated gas-solid phase mass transfer and due to an internally designed micro-scale water gradient promoting ion migration. Integrating this design into larger size devices, the voltage and current response similarly, highlighting, the potential suitability for scale up applications such as decorative lighting. Additionally, we demonstrated the feasibility of a novel coin battery-style MEG device, which delivered exceptional electrical generation performance with an output exceeding 3.8 V from a single unit. These results present a promising prospect for sustainable electricity generation through the regulation of ion migration in the local environment.

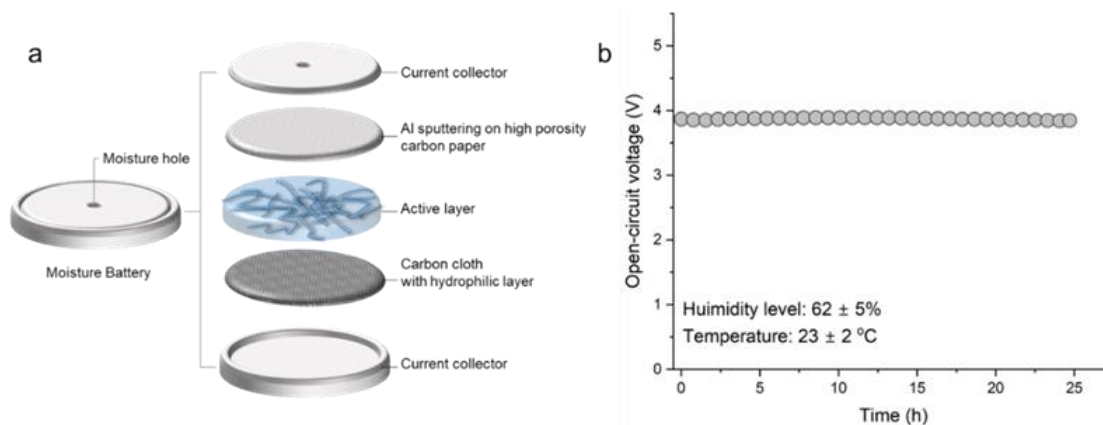


Figure 1: **a**, Scheme of coin battery-style MEG device. **b**, the open-circuit voltage output of the MEG device is sustained for over 25 h under atmospheric conditions.

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Two-dimensional ferroelectric materials on the applications of next-generation electronics

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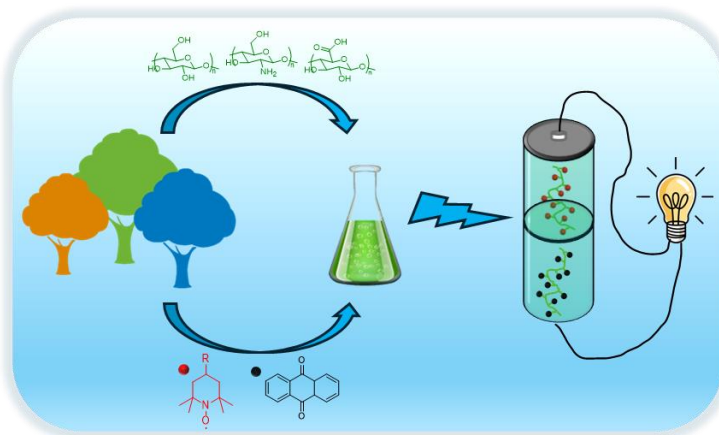
Effective manipulation for physical properties of nano-materials is fundamental for the development of next-generation electronic devices and has attracted numerous research interests. Two-dimensional (2D) ferroelectrics (FE) stand out as excellent candidates due to the promising properties of high density of storage and low-energy-consuming, which are expected to play an essential role in developing functional nano-scale electronic devices. In this presentation, by using the state-of-art density functional theory (DFT) and micromagnetic simulations, we systematically studied the impacts of stacking engineering and ferroelectric polarization on the physical properties of 2D materials, including GeSe/SnS heterobilayers, bilayer NiI₂ and monolayer CuCrP₂Te₆. The ultimate aim of this presentation is to manipulate the physical properties of 2D functional materials and explore the applications in electronics. The obtained knowledge is expected to guide and inspire experimental research and promote the development of nano-scale FE electronics.

Polysaccharide-based all-polymer rechargeable battery

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Global energy demand and consumption are escalating unceasingly due to increasing population and technological developments. The exploitation of renewable energy sources in the energy sector is rapidly growing, and energy storage systems (ESSs) have become a fundamental requirement. The common ESSs are rechargeable batteries, which mainly depend on heavy metals such as Li, Mn, Co, Ni, etc., for electrode active materials. However, the scarcity of resources and environmental hazards from disposed battery wastes influence finding of an alternative to traditional metal-based batteries [1]. Using redox-active polymers as electroactive materials for emerging organic energy storage represents an advance in reducing the dependency on rare and transition metals in ESSs. However, polymer-based ESSs mostly use non-degradable synthetic polymers which will cause new microplastic pollution [2][3], an existing issue yet to be resolved. Applying biopolymers could be a more sustainable approach to answering the drawbacks of current energy storage systems as these polymers are abundant in biomass and biodegradable [3][4]. To this end, we have successfully converted biopolymers into electrode-active materials through chemical modification with redox-active organic molecules, including TEMPO, anthraquinone, phenothiazine, viologen, etc. We demonstrated that these redox-active biopolymers could serve as electroactive materials and act as binders. Their hydrophilicity allows great applications in aqueous hybrid rechargeable batteries. The all-polymer battery will be a next-level approach in sustainable energy storage systems.



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Tunable Quantum Confinement in Individual Nanoscale Quantum Dots via Interfacial Engineering

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Introducing quantum confinement has shown promise to enable control of charge carriers. Although recent advances make it possible to realize confinement from semiclassical regime to quantum regime[1-6], achieving control of electronic potentials in individual nanoscale quantum dots (QDs) has remained challenging. Here we demonstrate the ability to tune quantum confined states in individual nanoscale graphene QDs, which are realized by inserting nanoscale monolayer WSe₂ islands in graphene/WSe₂ heterostructures, via interfacial engineering[7]. Our experiment indicates that scanning tunneling microscope (STM) tip pulses can trigger a local phase transition in the interfacial nanoscale WSe₂ islands, which, in turn, enable us to tune discrete quantum states in individual graphene QDs. By using a STM tip, we can also generate one-dimensional (1D) position-tunable domain boundaries in the WSe₂ islands. The 1D boundary introduces atomically wide electrostatic barriers that bifurcate quasibound states into two regions in the graphene QD, changing the QD from a relativistic artificial atom to a relativistic artificial molecule.

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Converting Industrial Polymer into Organic Cathode for Practical Aqueous Zinc-Ion Batteries

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Aqueous zinc ion batteries (AZIBs) are gaining significant attention due to their abundant resources and satisfactory safety profiles.[1] While much research has focused on optimizing the zinc anode, challenges remain in developing effective cathodes. Traditional metal oxide cathodes often suffer from low Zn^{2+} ion diffusivity, sluggish intercalation/deintercalation kinetics, and environmental concerns related to heavy metal ion hazards from spent batteries. In contrast, organic redox-active materials (ORMs) offer faster kinetics and reduced environmental impact, with polymeric ORMs presenting enhanced stability and processability.[2,3] However, current ORMs, particularly aromatic molecules and conducting polymers, are hindered by broad redox potentials, resulting in capacitance-like voltage outputs in AZIBs. Additionally, most ORM-based cathode studies remain at a conceptual stage, far from real-world application. We previously reported organic cathodes and identified TEMPO (2,2,6,6-tetramethylpiperidyl-1-oxy) radical as a promising candidate due to its high redox potential, stable redox reactions, and rapid electron transfer capabilities.[4] Despite these advantages, current polymeric TEMPO materials require complex synthesis processes, and the resulting AZIBs exhibit low mass-loading ($<1.5 \text{ mg/cm}^2$), limiting their practicality.

Here, we present a feasible synthesis method for a TEMPO-based polymer cathode derived from a low-cost industrial polymer.[5] This method enables the production of tens of grams of active polymer in the laboratory. We further evaluate the performance of organic AZIBs across various electrolytes, carbon additives, and battery fabrication conditions to minimize costs and environmental impact. The optimized AZIB delivers a discharge capacity of 92 mAh g^{-1} at 10C and operates at a voltage of 1.45 V. Remarkably, the battery retains 93% of its maximum capacity after 1000 cycles and maintains a Coulombic efficiency of 99.93%. Furthermore, by using ethanol as a solvent for slurry preparation, we achieve a mass loading of up to 50 mg/cm^2 , enabling the fabrication of 60-70 mAh pouch batteries capable of powering a model car and an electric fan. The material synthesis and cell fabrication conditions reported in this work mark a significant advancement in transitioning organic batteries from conceptual studies to real-world applications, contributing to sustainable energy storage solutions for millions of disposable electric devices.

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Electromechanical Energy Harvesting in Solvate Ionic Liquids and Advanced Electrolyte Systems

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Our research reveals how solvate ionic liquids (SILs) and epoxy-based polymer electrolytes generate voltage when compressed at pressures of up to 3.3 MPa [1]. Using lithium bis(trifluoromethanesulfonyl)imide solvated by triethylene glycol dimethyl ether, we demonstrate a novel piezoelectric-like effect where mechanical compression produces bulk potential differences. While previously observed in pure ionic liquids [2], we now show this phenomenon extends to their solvated forms and biphasic polymer electrolytes, generating voltages up to 150 mV and 45 mV, respectively.

Previously, our work showed that energy storage capacitance can be boosted via geometric manipulation of the device [3]. This stark increase was confirmed to be caused by the electromechanical charging effects in this work from the piezoelectric liquid – the SIL – on its own and entrapped within the nanostructure of the biphasic polymer electrolyte. Additionally, research is underway to confirm the contact electrification effects as the second cause of the increase in energy storage performance by simply changing the device shape, both of which were behind the self-charging effect observed previously.

Challenges were encountered particularly in the design and optimisation of the custom test setup required to ensure optimal conditions to contain and pressurise the SIL without forming a vacuum that prevented the depressurisation step and return to baseline. This discovery has significant implications for structural energy storage, particularly in applications where electrolytes undergo morphological changes. The ability to convert mechanical stress into electrical potential opens new possibilities for self-charging sensors, composite health monitoring, and enhanced energy storage efficiency through mass-less charging mechanisms.

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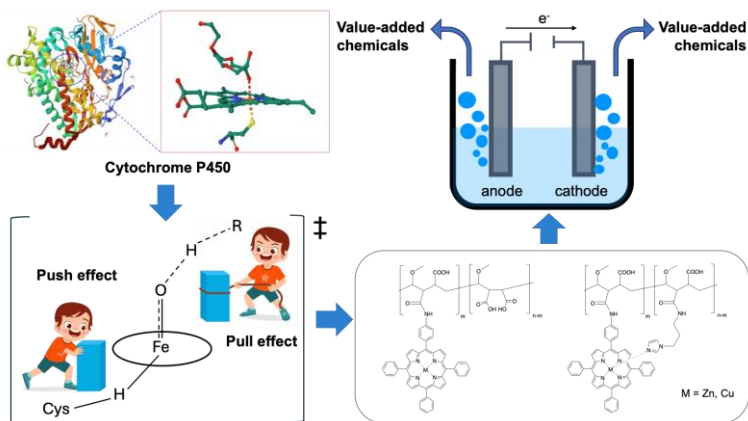
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Enzyme-Inspired Design of Polymer-Supported Catalysts for Applications in Electrocatalysis

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Catalysts play a pivotal role in modern chemical synthesis. Over decades, enzymes have been recognized as excellent catalysts for many artificial chemical reactions due to their high selectivity and efficiency. However, the direct use of natural enzymes in chemical synthesis faces multiple challenges, including their poor tolerance to harsh reaction conditions.[1] As such, designing catalysts that closely mimic the core structure of enzymes whilst being stable in various chemical reactions is of great importance. Metalloporphyrins are a common catalytic centre that exist in many redox-active enzymes. Specific amino acid residues can coordinate and render a push/pull effect to the metal centre to realize different catalytic activities.[2][3] Hence, metalloporphyrins with coordinated ligands have become prominent bio-mimicking catalysts. However, the microenvironment of these coordination structures remains far from that of the enzyme microenvironment. Herein, a polymer-supported metalloporphyrin catalyst was developed. *Poly(methyl vinyl ether-*alt*-maleic anhydride)*, an inexpensive polymer produced on an industrial scale, was modified with amino-functional metalloporphyrins and ligands. We demonstrate that the random-coil polymer chain facilitates coordination between the ligands and the metalloporphyrin. Meanwhile, the pendant carboxylic acid creates a hydrophilic microenvironment and can act as a proton-relay. Such a design takes a step closer to mimicking the active centre and microenvironment of redox enzymes. This polymer-supported catalyst is expected to enhance the electrochemical synthesis of H₂O₂, CO₂ reduction, or water splitting.



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Exploring bio-derived materials: using Thiol-Ene chemistry to expand bio-derived polymer applications

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More than 90% of today's synthetic polymers are derived from fossil fuels, 87% of these contribute to plastic waste. The largest source of renewable carbon-based energy is biomass waste. Cellulose accounts for up to 40-50 % of biomass waste. Biomass waste is a renewable source of valuable monomer and polymeric material. Chemical modifications of biomass waste products can yield desired scaffold monomers. The polymerised materials are viable alternatives to petrochemical derived polymers.[1]

The polymer latex market is also dominated by synthetic polymers, primarily produced from fossil-fuel based resources. Waterborne latexes are an important material used in the paints and surface coatings sector, and are also traditionally synthesized from petrochemical derivatives; bioderived latexes (or indeed latexes with a relatively high mass fraction of bioderived polymer) are therefore desirable to address both plastic sustainability concerns as well as to meet regulatory requirements. There is a demand to improve the accessibility of bioderived monomers, in particular making their synthesis attractive and commercially viable for use on an industrial scale.

The work herein, attempts to find an alternative to petrochemical derived polymers via the synthesis of monomers and polymers to create biobased plastics. Exploring a variety of applications from bio-derived 3D printing inks, surface coatings and recyclable polymer systems. A catalogue of monomer derivatives is readily available at hand, with selective, tailored chemical functionality.

The novel plastic materials have been examined for their rapid (<60s) cure kinetics, used to form cross-linked networks and analysed via mechanical analysis, thermogravimetric analysis (TGA).[2, 3] We have also report the ab initio thiol-ene emulsion polymerization of three bioderived diene monomers with a commercial dithiol, to prepare polymer latex particles using thermally initiated radical methods. The three diene monomers that we prepared are based on the chemical modification of LGA and LGO anhydrosugars derived from cellulose pyrolysis, as well as isosorbide, a diol produced from the dehydration of D-sorbitol. All generate stable polymer latexes via thiol-ene emulsion polymerization, with particle size related to the nature of the monomer employed.[4]

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Redefining Interfacial Solar Steam Generation: Harvesting Energy from Bulk Water for Ultra-High Evaporation Performance

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Interfacial solar steam generation (ISSG) is a promising and environmentally friendly technology for numerous applications, including seawater desalination, wastewater treatment, sterilization, power generation, and soil remediation [1-2]. ISSG systems have the capability to convert sunlight into thermal energy to generate vapor on the evaporation surfaces, and the evaporation rates are determined by the energy conversion and utilization efficiencies. Compared with two-dimensional (2D) ISSG systems, where sunlight is the only energy source, 3D ISSG can harvest additional energy from air and bulk water to reach a higher evaporation performance. Due to the high heat capacity of water, bulk water has the potential to replace solar energy as the dominant energy source for photothermal water evaporation, thus realizing all-day highly efficient water evaporation and clean water production [3]. Here, to further enhance the energy extracted efficiency from bulk water, a series of copper evaporator supports with fins were prepared to connect evaporation surfaces and bulk water. Due to high thermal conductivity and large contact area, the newly designed evaporators demonstrate an excellent energy extraction capacity from bulk water, leading to remarkably high evaporation rates up to $11.15 \text{ kg m}^{-2} \text{ h}^{-1}$. Calculation and simulation results prove that the harvested energy from bulk water by the evaporator is about 24.8 times greater than the solar energy input. This finding highlights that bulk water is the vast energy reservoir in ISSG, which has been previously overlooked. By harvesting energy from bulk water, evaporation performance reaches unprecedented levels, suggesting a potential model shift in designing future 3D photothermal evaporators, with bulk water as the primary energy source.

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The Structure and Dynamics of Supercritical CO₂: A Recent Theoretical Investigation

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This presentation delves into the structure and dynamics of supercritical carbon dioxide (sCO₂), focusing on its recent theoretical investigation. sCO₂, formed above its critical temperature (304.13 K) and pressure (73.8 bar), exhibits unique physical properties that blend liquid-like density with gas-like diffusivity. These properties make it a versatile medium for numerous industrial applications, including power generation, carbon capture, and chemical processing. The presentation explores classical molecular dynamics (MD) simulations, which have significantly advanced our understanding of sCO₂'s microstructure and transport behavior. Additionally, it highlights the role of quantum chemical methods, particularly ab initio molecular dynamics (AIMD), in providing deeper molecular insights. Through this examination of theoretical models, we gain a comprehensive understanding of how sCO₂ behaves at the microscopic level and how its structure and dynamics influence its performance in industrial contexts. This investigation is essential for optimizing sCO₂-based technologies, with implications for energy efficiency and environmental sustainability.

Interfacial Photothermal Evaporation and Applications

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Freshwater is essential for sustaining human survival and development. According to the WHO, billions of people around the world currently face drinking water shortages.^[1] To address this challenge, various water purification technologies have been developed.^[2] Among them, the recently developed interfacial solar evaporation (ISE) technology offers a more sustainable and cost-effective solution for clean water production by harnessing solar energy.^[3-5] Over the past decade, significant efforts have been devoted to optimizing the overall performance of ISE.^[6-10] These include the exploration of photothermal materials to improve light-to-heat conversion, advanced structure design of evaporator to enhance energy management, and the development of innovative fouling-resistant evaporators for sustainable desalination.

Despite these achievements, there remains potential to further improve ISE systems, particularly in purifying complex water sources for practical, real-world applications.

This presentation aims to provide a clear introduction to ISE technology for a broad audience. It will begin with an overview of the fundamental working principles of ISE, followed by strategies to optimize energy utilization and address challenges related to salt accumulation. The final section will highlight real-world applications of ISE, showcasing its promising potential for widespread use.

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Aggregation Suppression and Enhanced Blue Emission in a Coordination Polymer Glass Composite

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High-efficiency and operationally stable blue-emitting organic light-emitting diodes (OLEDs) are essential for advancing solid-state lighting applications.^{1, 2} Perylene, a blue luminescence organic dye known for its high luminescence efficiency, holds great potential for fabricating emitting diodes. However, a major obstacle is the aggregation-caused quenching (ACQ) effect, which remarkably reduces its efficiency and causes redshifts in photoluminescence emission.^{3, 4} Overcoming ACQ and enhancing material stability is crucial in the fabrication of OLEDs. Herein, we successfully fabricated blue-emitting coordination polymer glasses by integrating perylene dye with a zinc-based coordination glass. This approach effectively suppressed the J-aggregation, which occurs when perylene monomers stack in parallel in the solid state. Moreover, the hybrid glass demonstrated high stability and strong photoluminescent quantum yield (PLQY) under ambient conditions. Given its strong PLQY, stability and transparency, this approach offers a promising pathway for developing semi-transparent hybrid composite glasses using other organic dyes that face similar challenges.

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Metal-organic framework glass composite membrane for H₂ purification

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Abstract:

Hydrogen as a clean energy carrier with high energy storage capacity, is regarded as an important green secondary energy source in sustainable development, and it is predicted that hydrogen energy will be responsible for 18% of global energy end-use demand by 2050^[1]. At present, the hydrogen production mainly sources from reforming fossil energy, but substantial amount of CO₂ and other by-products are released in the process of producing hydrogen, thus H₂ purification and separation is an important step to produce clean energy and reduce greenhouse gas emissions^[2]. Membrane-based H₂ purification technology becomes the candidate on account of its simplicity and energy-efficient. Metal-organic frameworks (MOFs) have been used to combine with membrane separation technology to achieve enhancement of gas separation due to their high porosity and structural tunability. However, the grain boundary defects between MOF crystal particles give rise to the difficulty in fabricating a membrane with a certain thickness and retaining the independent integrity at the same time. In recent years, a melted liquid state of MOFs, namely MOF glass, has been widely studied as the unique physical and chemical properties of MOF glass strengthen its processability. However, some self-supported MOF glass membranes (e.g., ZIF-62 and ZIF-4) are unable to achieve high gas permeability, then promoting the development of crystal-glass composites (CGC) to increase gas permeability and strengthen the mechanical property. In this study, g-C₃N₄ as a two-dimensional material with abundant nanochannels, was selected as the dispersed phase to form a CGC membrane in which the glassy ZIF-62 acts as continuous phase. The composite membrane improved the interfacial properties with the assistance of g-C₃N₄ surface functional groups; additionally, continuous and efficient pathways induced by melting-quenching were generated in the membrane to achieve efficient H₂/CO₂ separation of 9.53 and exhibit a high H₂ permeance of 68610 Barrer. This work not only provides a new method for the preparation of self-supported CGC gas separation membranes, but also have important implications for the development of separation membrane materials with good interfacial compatibility and overcome trade-off effect.

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Multifunctional Lead-Free Metal Halide Perovskite Modified electrolyte for High-Performance Aqueous Zinc-ion Batteries

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Aqueous zinc-ion batteries (AIZBs) offer a safer and more sustainable alternative to traditional batteries, but they face challenges such as dendritic growth, self-corrosion, hydrogen evolution reaction (HER), and passivation layer formation, which limit their performance and lifespan. Electrolyte engineering has emerged as a practical and cost-effective method to address these issues by stabilizing the anode-electrolyte interface. Various additives, including proteins, polymers, and inorganic materials [1], have been developed to promote nucleation, suppress dendrite growth, and optimize solvation structure, but most only address one or two aspects of the battery performance.

Metal halide perovskites (MHPs) have primarily been used in solar cells due to their excellent light absorption and charge-carrier mobility. However, their use in zinc-ion batteries, particularly as electrolyte additives, remains largely unexplored. Their adaptable chemical compositions and unique lattice structures present opportunities to improve battery efficiency and longevity.

In our study, we introduce a Lead-Free metal halide perovskite as a multifunctional electrolyte additive for AZIBs, providing four key benefits. These include modifying the solvation structure to reduce side reactions, assisting in the nucleation process for more uniform Zn deposition, preventing dendrite growth through a protective mechanism, and stabilizing the pH during battery cycling to minimize fluctuations and side reactions. These combined effects contribute to overall improved battery performance and longevity.

Experiments show that the multifunctional perovskite additive significantly improves battery performance. In symmetric cells, stable cycling was achieved for over 5000 hours, while full cells retained over 80% of their capacity after 1000 cycles. These results underscore the effectiveness of the metal halide perovskite additive in improving both electrolyte stability and electrode performance.

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SiC substrate-enabled modulation of Li⁺ ion intercalation thermostability in strained bilayer graphene

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Two-dimensional (2D) van der Waals (vdWs) materials have emerged as vital components in various technological fields. Ion intercalation into vdWs materials is a versatile technique for materials exfoliation, properties induction, and stacking order manipulation. However, the role of the substrate and its consequential impact on ion intercalation thermodynamics in vdW materials is yet to be well understood. In this work, employing density functional theory (DFT) calculations, we investigate the interplay between the SiC substrate and Li⁺ ion intercalation in the strained bilayer graphene grown on the SiC (0001) substrate. Our analysis covers five stacking orders (AA, AB, BA, SP, and IM stacking), revealing that the SiC substrate enhances the thermostability of Li⁺ ion intercalation. This enhancement is attributed to the special *sp*³-hybrid carbon atoms in the bottom graphene layer. We observed that the SiC substrate promotes selective intercalation with stacking preference, favoring AA stacking over the other four stackings. Surprisingly, the SiC substrate disrupts the crystal symmetry within bilayer graphene, leading to distinctive intercalation behaviors in AB and BA stackings that are absent in the free-standing bilayer graphene. Our study offers a comprehensive understanding of the intricate relationship between substrates and ion intercalation in layered materials, thereby paving the way for tailored applications of layered vdW materials with substrates through ion intercalation.

Interlayer Interaction Arising from Lone Pairs in s-Orbitals in 2D Materials

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Interlayer interactions or hybridization in van der Waals (vdW) heterostructures of two-dimensional (2D) materials significantly influence their physical characteristics, including layer-dependent electronic and vibrational structures [1], magic-angle superconductivity [2], interlayer antiferromagnetism [3], and interlayer excitons [4]. These interactions are sensitive to a set of interdependent and externally tunable parameters. To fully exploit the potential of these materials, it is crucial to understand the physical origins of interlayer interaction and hybridization. Traditional theories often attribute these interactions to the sharing of electrons via p orbital lone pairs or π electrons [5], based on the octet rule, which posits that p electrons are the primary occupants of the outermost atomic shells, except in hydrogen. However, our study challenges this prevailing belief. Through high-throughput screening, we demonstrate that s orbital lone pairs can also drive interlayer interactions in 2D materials. The crystal field and inert pair effect induce a Stark-like phenomenon, leading to energy level splitting and the formation of directional electron clouds. This allows these electrons to directly participate in the hybridization of interlayer wavefunctions without forming chemical bonds. Our findings expand the understanding of interlayer interactions, revealing new mechanisms that govern these properties and providing a theoretical foundation for manipulating interlayer phenomena in 2D materials.

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Covalent organic framework coated with coordination polymer glass for high-efficiency selective CO₂ capture

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Excessive carbon dioxide (CO₂) emissions have led to climate change, ocean acidification and health risks, becoming a major environmental and public health issue [1]. Selective capture of CO₂ from emission sources, such as power plant flue gases, is critical to recovering C1 resource. Covalent organic frameworks (COFs) are widely used in gas storage as a promising platform for porous materials, owing to their advantages of good chemical stability, large specific surface area, low density and regular pore structure. The porosity of COF enables significant gas adsorption, but their large pore sizes often hinder selective separation efficiency.

Post-modification of covalent organic frameworks (COFs) has become a cutting-edge approach for enhancing CO₂ selective capture. Few capture systems of this sort have been exploited, as their rigid frameworks require long synthesis time (usually exceeding 72 h), are susceptible to collapse upon introducing moieties and pose challenges for their integration [2].

Recent research has revealed coordination polymer (CP) with solid-liquid transition capability [3], which we utilize here to create efficiently synthesized, stable, functional and porous composite materials. Thus, a series of highly crystalline (agZnCP)_X-(TPP-COF)_{(1-X)%} is rapidly synthesized within 8 hours by the aid of N₂ activation and CP glass (agZnCP) fixation, significantly enhancing the synthesis rate. The covalent bonds and chemical structure of the TPP-COF crystalline phase are maintained within the agZnCP matrix. Moreover, the interfacial interaction between the closely contacted microdomains enhance the crystallinity of TPP-COF. The agZnCP coated on the TPP-COF skeleton with nanoscale regular channels ensures an even distribution of micropores on the glass surface and effectively reduces the pore size of the COF, which are advantageous for CO₂ gas molecular diffusion, enrichment, and selective adsorption. We find that there is a contradictory balance between the coating amount and pore size of TPP-COF. The CO₂/N₂ selectivity of (agZnCP)₄₅-(TPP-COF)₅₅ (28.11) improved by 34% compared to that of individual TPP-COF (20.97) (Figure).

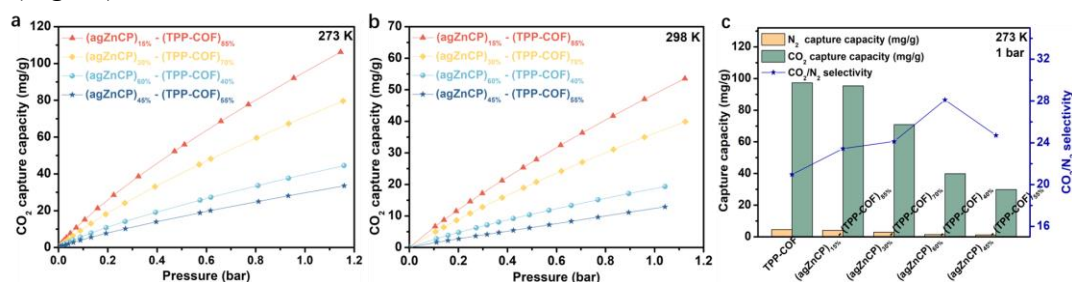


Figure. CO₂ adsorption isotherms of (agZnCP)_X-(TPP-COF)_{(1-X)%} at (a) 273 K and (b) 298 K. (c) ideal CO₂/N₂ selectivity of (agZnCP)_X-(TPP-COF)_{(1-X)%}.

Keywords: Covalent organic framework; Coordination polymer glass; Enhanced crystallinity; CO₂/N₂ selectivity

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Coordination Polymer Liquid Crystal and Glass

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Liquid and glassy coordination polymers (CPs) and metal–organic frameworks (MOFs) have demonstrated great potential in a wide range of fields such as molecule separation and proton conductivity. However, most meltable CP/MOF materials will lose their crystalline structure upon surpassing their melting point during the solid-to-liquid phase transition. Here, we present a novel thermotropic ZnCP liquid crystal (LC) material, composed of zinc ions, benzimidazole, and phosphate, which retains its crystalline structure even after melting. This ZnCP can self-assemble into a kind of LC nanostructures through phase segregation, driven by hydrogen bond and intermolecular interactions. This unique combination of the good fluidity and long-range order results in a highly distinctive material, which can be used as one of promising electrolyte candidates. X-ray techniques were used to investigate the structural evolution of the ZnCP during its transitions from crystal to LC, and eventually to glass. Thermodynamic analysis revealed that this ZnCP had a low melting point of about 125°C, and the LC phase had ultrahigh stability at 150°C based on the abundant hydrogen bond between zinc phosphate and benzimidazole. Morphological and lattice changes were further analysed using scanning and transmission electron microscopy. Remarkably, the ZnCP LC preserves its crystalline structure upon cooling after melting. Proton conductivity measurements revealed that the ZnCP LC exhibited enhanced performance compared to its unmelted crystalline and glass phases, particularly at low temperatures. This newly discovered LC material, based on coordination networks of metal ions/clusters and organic ligands, will offer a new route to design advanced ion transport systems for modern electrochemical and electronic devices, such as developing high-performance liquid-crystalline electrolytes.

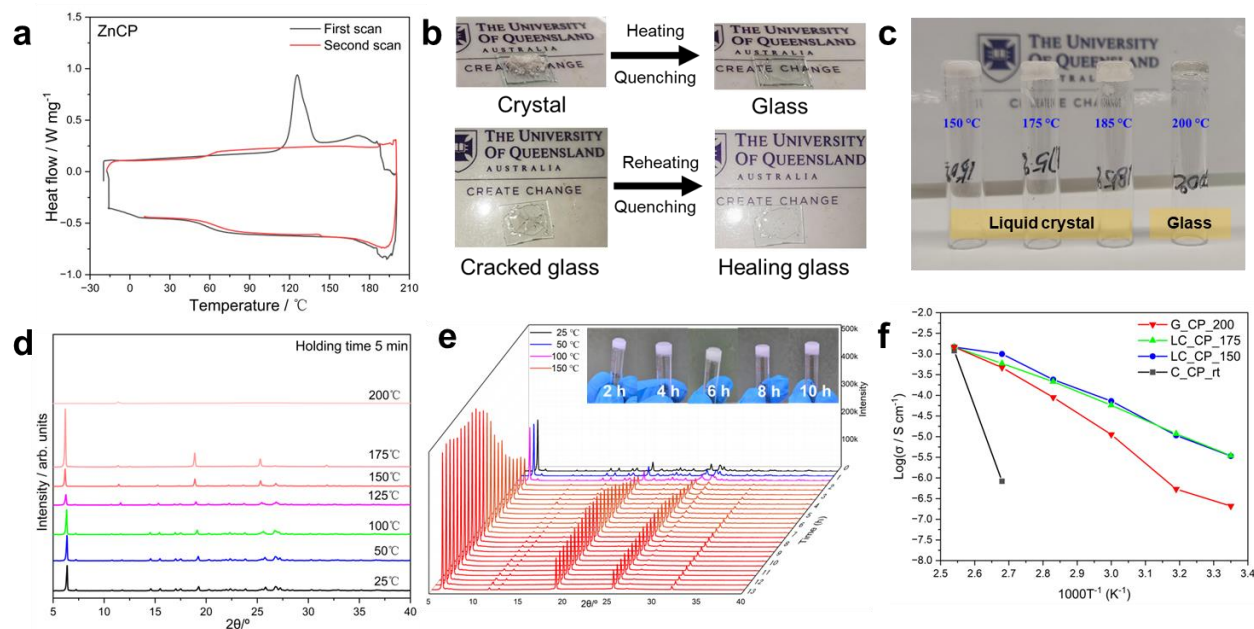


Figure 1 (a) Differential scanning calorimetry (DSC) curves of ZnCP under Ar flow. (b) Photographs depicting the melting process of ZnCP into a glassy state, as well as the self-healing of cracked ZnCP glass upon heat treatment. (c) Optical images of ZnCP at different temperatures with holding time 30 minutes under flowing Ar, (d) Variable-temperature powder X-ray diffraction (VT-PXRD) pattern of ZnCP under flowing N₂, (e) VT-PXRD pattern of ZnCP at 150°C from 1h to 10h under flowing N₂, (f) Variable temperature anhydrous H⁺ conductivity for different ZnCP.

Bioinspired design and application in aqueous Zn-ions battery

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Aqueous Zn-ion batteries (AZIBs) have been regarded as a promising candidate for next generation energy storage, due to their attractive high safety and low cost. However, the grand challenges resulting from undesired side reactions, such as dendrite growth, hydrogen evolution reaction (HER), and self-corrosion, have retarded their real-world applications. While significant progress has been achieved in solving these challenges in AZIBs, a comprehensive understanding of designing high-performance and robust Zn-ion-based batteries is urgently demanded.

In the first case, inspired by the regulated nucleation and growth of inorganic minerals from a porous organic matrix within the biomineralization process, dopamine-derived N-doped carbon spheres with abundant gaps and voids are assembled onto the Zn metal anode (Zn@C) as an artificial solid electrolyte interphase (SEI) layer to modulate the nucleation and growth of a smooth Zn layer without dendrites and suppress the corrosion and hydrogen evolution side reactions. When assembled into Zn-ion batteries, the bioinspired electrode presents comprehensive enhancements in terms of capacity, rate performance, and stability. This unique design of electrode allows long-term stable cycling up to 2,100 h at 5 mA cm⁻² for a symmetric battery and gives rise to the performance of 315 mAh g⁻¹ at 0.5 A g⁻² and 95% retention of its original capacity after 1,000 cycles for the Zn@C//V₂O₅ pouch cell, which outperform most of reported Zn electrodes [1].

In the second case, inspired by the ultra-fluidic and K⁺ ion-sieving flux through enzyme-gated potassium channels (KcsA) in biological plasma membranes, a metal-organic-framework (MOF-5) grafted with -ClO₄ groups as functional enzymes is fabricated to mimic the ultra-fluidic lipid-bilayer structure for gating Zn²⁺ “on” and anions “off” states. Resulting from the perfect Zn²⁺/SO₄²⁻ selectivity (~10), enhanced Zn²⁺ transfer number ($t_{Zn^{2+}} = 0.88$) and the ultra-fluidic Zn²⁺ flux (1.9 × 10⁻³ mmol m⁻² s⁻¹ vs. 1.67 × 10⁻³ mol m⁻² s⁻¹ for KcsA). The symmetric cells achieve a lifespan of over 5,400 h at 10 mA cm⁻²/20 mAh cm⁻². Specifically, the performance of the PMCl-Zn//V₂O₅ pouch cell keeps 81% capacity after 2,000 cycles at 1 A g⁻¹[2].

In the third case, introducing catechol (CAT) into the aqueous electrolyte, an outer sphere electron transfer mechanism is intrigued to inhibit the water reactivity, achieving an electrochemical window of 3.24 V. In a typical Zn-ion battery, the outer sphere electrons jump from CAT to Zn²⁺-H₂O at a geometrically favorable situation and between the complexes without breaking or forming chemical bonds as that of the inner sphere electron transfers. The excited state π - π stacking further leads to the outer sphere electron transfer occurring at the electrolyte/electrode interface. This high-voltage electrolyte allows an operating voltage two-times higher than the usual aqueous electrolytes and provides almost the highest energy density and power density for the V₂O₅-based aqueous Zn-ion full batteries. The Zn//Zn symmetric battery delivers a 4,000 h lifespan, and the Zn//V₂O₅ full battery shows a ~380 Wh kg⁻¹ energy density and a 92% capacity retention after 3,000 cycles at 1 A g⁻¹ and 2.4 V output voltage [3].

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Realization of $\frac{2}{3}$ -layer transition metal dichalcogenides

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Layered van der Waals transition metal dichalcogenides (TMDCs), generally composed of three atomic X-M-X planes in each layer (M = transition metal, X = chalcogen), provide versatile platforms for exploring diverse quantum phenomena [1]. In each MX₂ layer, the M-X bonds are predominantly covalent in nature, as a result, the cleavage of TMDC crystals always occurring between the layers [2]. Here we report the controllable realization of fractional-layer WTe₂ via an in-situ scanning tunnelling microscopy (STM) tip manipulation technique. By applying STM tip pulses, hundreds of the topmost Te atoms are removed to form a nanoscale monolayer Te pit in the 1T'-WTe₂, thus realizing a brand-new $\frac{2}{3}$ -layer WTe₂. Such a unique configuration undergoes a spontaneous atomic reconstruction, yielding an energy-dependent unidirectional charge-density-wave state with the wavevector and geometry quite distinct from that of pristine 1T'-WTe₂. Our results expand the conventional understanding of the TMDCs and are expected to stimulate the research on extraordinary structures and properties based on fractional-layer TMDCs [3].

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Fractional quantum Hall effect in n-type semiconductor MoS₂

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Finding methods or material systems to achieve high-mobility two-dimensional semiconductors is an important research direction in condensed matter physics and even nanoelectronics.

It is well known that since the discovery of the quantum Hall effect in high-mobility two-dimensional electron gases in quantum wells over 40 years ago, the realization of the quantum Hall effect or fractional quantum Hall effect in two-dimensional electron systems remains very limited. Among them, the low-temperature ground state of high-mobility two-dimensional semiconductors is particularly difficult to realize, mainly due to the extremely challenging acquisition of Ohmic contacts.

In this talk, we will introduce the latest progress in the stable and reliable preparation of low-temperature Ohmic contacts in n-type molybdenum disulfide field-effect transistors, where the quantum limit (filling factor of $\nu=1$) can be achieved, and fractional quantum Hall effect (FQHE) with fillings of $2/5$ and $4/5$ under mK temperatures are observed [1]. This is the first two-dimensional n-type semiconductor material where the FQHE can be observed through electrical transport (excluding those topological flat band systems). Our results of ultra-high mobility n-type MoS₂ layers pave the way for TMD-based transistors for future nano-electronic devices at cryogenic temperatures.

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Modeling Critical Thermoelectric Transports Driven by Band Broadening and Phonon Softening

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Critical phenomena are one of the most captivating areas of modern physics, whereas the relevant experimental and theoretical studies are still very challenging. Particularly, the underlying mechanism behind the anomalous thermoelectric properties during critical phase transitions remains elusive, i.e., the current theoretical models for critical electrical transports are either qualitative or solely focused on a specific transport parameter. Herein, we develop a quantitative theory to model the electrical transports during critical phase transitions by incorporating both the band broadening effect and carrier-soft TO phonon interactions [1]. It is found that the band-broadening effect contributes an additional term to Seebeck coefficient, while the carrier—soft TO phonon interactions greatly affects both electrical resistivity and Seebeck coefficient. The universality and validity of our model are well confirmed by experimental data. Furthermore, the features of critical phase transitions are effectively tuned. For example, alloying S in Cu₂Se can reduce the phase transition temperature but increase the phase transition parameter b . The maximum thermoelectric figure of merit zT is pushed to a high value of 1.3 at the critical point (377 K), which is at least twice as large as those of normal static phases. This work not only provides a clear picture of the critical electrical transports but also presents new guidelines for future studies in this exciting area.

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Glassy metal-organic framework (MOF) composite membranes for gas separation

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Abstract

The separation and purification of gases are requisite industrial processes necessary to attain specific product standards and purity levels in energy and chemical production industries [1]. Currently, gas separation primarily relies on traditional techniques such as cryogenic distillation and chemical absorption, which not only generate pollution but also consume a great deal of energy across the globe [2]. Compared with other conventional gas separation strategies, the membrane-based gas separation process has been extensively studied because of its inherent advantages such as reduced carbon and energy footprints, high energy efficiency, ease of fabrication and scale-up, and cost competitiveness [3]. Among various membrane materials, mixed matrix membranes (MMMs) are recognised as a standout option which can overcome the permeability-selectivity trade-off limitations that are commonly observed in normal polymer membranes by leveraging both the properties of the polymeric matrix and the advantages of porous fillers [4, 5]. Inspired by this, this study developed the MMM by using nano-sized porous glassy MOFs with phase transition properties as fillers. The CO₂ permeability as well as the CO₂/CH₄ and CO₂/N₂ selectivity of MOF-loaded membranes were significantly increased by 40% compared with the pure polymer membrane. The MMM overcame the trade-off effect based on the porosity of the loaded MOF and the good compatibility within the interfacial regions between the MOF and polymer phase. Furthermore, the effect of thermally-induced phase transition of MOF glass on membrane gas separation performance was investigated. After *in situ* heat treatment, glass-based MMM showed enhanced CO₂ permeability with no obvious decrease in CO₂ selectivity. This research demonstrates an advance in improving the interfacial compatibility within the MMM and provides a promising direction for the rational design of MOF glasses-loaded MMMs with high gas separation performance.

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An Investigation into Biomimetic Structures Inspired by Plants

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Throughout the extensive timeline of history, organisms in nature have gradually evolved to develop a series of specialized protective structures. These intricate structures typically exhibit exceptional strength, modulus, toughness, and other functional attributes, providing valuable inspiration for human innovation in the design and fabrication of high-performance components. In recent decades, significant advancements have been made in the exploration, development, and application of biomimetic structures ^[1-6]. Notably, both plant and animal architectures have garnered increasing attention across various fields due to their promising potential.

This study aims to investigate the inspirational role of plant microstructures in biomimetic structural design, particularly concerning their prospective applications within materials science and engineering. Through a comprehensive literature review coupled with experimental analysis, we examined the microstructural characteristics of diverse plant types; these characteristics encompass cell arrangement patterns, wall thicknesses, and pore size properties. Furthermore, these findings were integrated with principles from materials science; appropriate software was utilized to simulate the mechanical response behaviors of biomimetic structures inspired by these plant features while exploring their specific applications within engineering contexts.

The research results indicate that leveraging insights from plant microstructural architecture can significantly inform the design and production of novel high-performance materials. For instance, certain biomimetic structures derived from plant tissues demonstrate outstanding mechanical properties such as compressive strength and tensile strength alongside advantageous functional traits like lightweight construction.

In conclusion, this study posits that a profound understanding and application of plant morphology will yield substantial benefits for future engineering practices aimed at fostering human innovation. By promoting interdisciplinary collaboration that integrates natural wisdom into contemporary technological solutions is anticipated to enhance efficiency while ensuring environmental sustainability—providing new strategies for addressing complex engineering challenges.

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Concentration Gradient Hydrogel Electrolyte Enhance Rapid Ion Transportation to Improve Aqueous Zinc-ion Batteries

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Rechargeable aqueous zinc-ion batteries attract significant attention due to their low cost, high safety, substantial theoretical capacity (820 mAh g⁻¹), and low redox potential (-0.76 V vs. SHE) [1]. Nonetheless, they face considerable challenges, including dendrite growth, the hydrogen evolution reaction (HER), and uncontrolled passivation reactions [2]. Hydrogel electrolytes present a promising solution to mitigate these issues by inhibiting dendrites and byproducts. However, a trade-off exists between the polymer content and ionic conductivity within hydrogel electrolytes. Herein, this work introduces a concentration gradient hydrogel electrolyte (GHGE) offering high ionic conductivity at low concentrations, enhanced physical properties, and dense zinc deposition at elevated concentrations. The asymmetric concentration distribution within the GHGE facilitates fast and selective ionic transport, achieving a Zn²⁺ transference number of 0.88. Furthermore, the high-density hydrogels effectively immobilize free water and ensure a uniform Zn²⁺ flux, resulting in flat and dense zinc (002) deposition. Consequently, the GHGE demonstrates the capacity for Zn stripping/plating over 2500 hours at current densities of 1 mA cm⁻² and 1 mAh cm⁻², significantly extending the cycle life in various full battery configurations. This research paves the way for the development of concentration gradient electrolytes.

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POSTER PRESENTATION

Photoinduced decomposition mechanism in 2D perovskite

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Halide perovskite quantum wells, also known as 2D perovskites respecting a chemical formula of $L_2A_{n-1}Pb_nX_{3n+1}$ (L is organic ligand; A is Cs^+ , $CH_3NH_3^+$, or $CH(NH)NH_3^+$; B is Pb^{2+} or Sn^{2+} ; X is Cl^- , Br^- , or I^-), are an emerging optoelectronic material that has been attracting increasing research attention. Their anisotropy and quantum confinement effect endow unique optoelectronic properties. Besides, they also offer a coherent 2D/3D perovskite interface that is widely applied for improved optoelectronic device performance. However, 2D perovskites suffer from photo instability, and the underlying mechanism is still unclear. We found that ultraviolet photons could pump electron transition from the organic ligands to the lead halide sublattice, subsequently driving deprotonation of the ammonium group in the organic ligand. Such deprotonation of the ammonium group breaks the bonding of the ligand to the lead halide sublattice and therefore causes decomposition of 2D perovskites. The discovery of the mechanism underlying the photo-instability of 2D perovskites could inspire countermeasures and promote their optoelectronic applications.

Towards the synthesis of a novel carbon fibre reinforced vitrimer composite

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Since their discovery in 2011, vitrimer materials have emerged as a solution to the limitations of both thermosets and thermoplastics. These materials have a structure that consists of a three-dimensional covalent network, similar to a thermoset, but they feature dynamic covalent bond exchange when exposed to elevated temperatures. This unique property gives vitrimers the high specific strength and stiffness characteristic of thermosets at standard working temperatures while enabling reshaping, healing, and recycling at higher temperatures. Research on applying vitrimers in fibre-reinforced composites remains limited yet offers significant potential [1].

This project aims to develop innovative approaches for integrating vitrimer materials between a base resin and carbon fibers to create high-stiffness structural composites with enhanced resistance to delamination. The Hooper and Henderson group has pioneered a silver-catalysed decarboxylative method for grafting polymers onto graphitic surfaces. In this project, we propose grafting a modified epoxy polymer onto carbon fibre, which can then be rendered vitrimeric through a silver-catalysed radical decarboxylative process [2].

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Membrane-Free Water Electrolysis for Hydrogen Generation with Low Cost

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Electrolysis of water to produce H₂ is the most promising technology to solve global energy crises because it can be performed under ambient conditions using electricity from sustainable wind and solar energy sources. However, the cost of H₂ produced by conventional proton exchange membrane water electrolyser (PEMWE) or alkaline water electrolyser (AWE) is much higher than that generated from reforming fossil fuels (*ca.* \$4.00-9.00 vs. \$2.50 kg⁻¹). At present, the cost of green H₂ is limited mainly by expensive membrane-electrode assemblies and sluggish oxygen evolution reaction (OER) at the anode. To attenuate membranes degradation or eliminate the need for membranes, the concept of decoupled water electrolysis was recently developed. Although this strategy is promising for membrane-free electrolysis and reducing the risk of H₂ and O₂ mixing, it is limited by unsatisfactory Faradaic efficiency (*ca.* 68%) of H₂ evolution and lower electrolysis efficiency. On the other hand, to solve the issue of sluggish OER, some research works reported thermodynamically favourable small molecule oxidation reactions (e.g., urea oxidation, alcohol oxidation, glycerol oxidation, etc.) to replace OER for achieving a reduced operating voltage of electrolyser. Among these small molecule substrates, urea from wastewater or urine stands out due to its lowest energy cost and low equilibrium potential ($E^0 = 0.37$ V) for urea oxidation (UOR). Therefore, using UOR as the anode to develop novel membrane-free electrolysis systems would provide promising opportunities for low-cost H₂ production.

Conventional UOR usually proceeds in alkaline conditions, with Ni-based materials as the only catalysts. Unfortunately, these Ni-based UOR catalysts generate toxic NO₂⁻/NO₃⁻ rather than N₂, causing secondary environmental pollution. If operating in a membrane-free water electrolysis system, the NO₂⁻/NO₃⁻ on Ni-based catalysts may diffuse through the electrolyte to the cathode and compete with hydrogen evolution reaction (HER) via NO₂⁻/NO₃⁻ reduction reaction (NORR), which reduces the selectivity of desired H₂. Therefore, all reported urea-assisted water electrolysis must be equipped with anion exchange membranes. In addition, high-valent (Ni³⁺/Ni⁴⁺) active species on Ni-based catalysts simultaneously trigger competing OER, which cannot avoid the mixing of H₂ and O₂, significantly limiting the reliable construction of membrane-free systems. Therefore, it is important to develop alternative UOR catalysts with environmentally benign products (e.g., N₂) and OER inertness to replace conventional Ni-based catalysts, which is the key to achieving membrane-free water electrolysis for safe and low-cost H₂ production.

Here, for the first time, an efficient and robust membrane-free water electrolysis system was developed over a class of Cu-based UOR catalysts. Cu_xO exhibits ~100% UOR selectivity and 82.62% N₂ product selectivity (4 times higher than that of conventional Ni-based UOR catalysts) without any O₂. This ensures ultra-high H₂ Faradaic efficiency (above 90%) in the membrane-free two-electrode single-cell system constructed with Cu_xO anode, avoiding the hazardous issue of H₂ and O₂ mixing and mitigating the NORR competitive reaction. A series of in situ spectroscopic characterizations reveal that the unique N₂ selectivity and OER inertness on Cu_xO are attributed to a novel hydrazine-like *N₂H_y intermediate-mediated UOR mechanism, which is significantly different from the NO₂⁻/NO₃⁻ generation mechanism observed on Ni-based UOR catalysts. To validate and scale up this system, we assembled an industrial-type membrane-free water electrolyser (MFE) that reduces the electricity consumption from 5.17 kWh Nm⁻³ (commercial AWE) to 3.78 kWh Nm⁻³, thereby saving 26.89% of electricity. The elimination of the membrane requirement and the significant electricity savings successfully enable the MFE plant to produce H₂ at a lower cost (US\$1.81 kg⁻¹) than grey H₂ (US\$2.50 kg⁻¹), highlighting the economic feasibility and practicality of our membrane-free system.

Regulation of Carrier Dynamics in Metal Halide Perovskite for Light Emission Application

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The Ruddlesden-Popper perovskites are recognized as the most promising candidate for industrialized optoelectronic applications, due to their higher stability and lower defect density compared with the three-dimensional counterparts. The relationships on the self-assembled properties of multiple quantum wells in Ruddlesden-Popper perovskite and desired charge carrier funneling process in these materials, however, have not been extensively studied. Therefore, toward the application of quasi-two-dimensional perovskite in light emission, the crystallization kinetics of polycrystalline films, the regulation of quantum wells distribution and the charge carrier dynamics along the energy landscape were systematically investigated.

Firstly, we developed the strategies for regulating the crystallization kinetics of perovskites by utilizing the intermolecular forces, to achieve purposefully control of the carrier transmission dynamics; ^[1-2] Secondly, we constructed a funnel-type multi-quantum-well perovskite structure to modulate the carrier dynamics undergoing two-step energy relaxation to the luminescent center, and realize a dual-pulsed amplified spontaneous emission, which offering a new method for manipulating ultra-short laser pulses. ^[3-4] Thirdly, through regulating the carrier transfer process and the ratio of luminous centers in mixed dimensional perovskite films, the highly efficient and stable green light perovskite light emitting diodes was obtained. ^[5-6] These works provide great insights for the development of new-type and efficient light emitting applications.

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Enhanced Ion Selectivity in Vanadium Redox Flow Batteries Using Acid-Etched Graphene Oxide Hybrid Membranes

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The permeation of vanadium ions across the membranes is the main reason contributing to the low energy efficiency and high capacity fading of vanadium redox flow batteries (VRFB). Here, a high-performance sandwich-structured hybrid membrane for VRFB have been developed, employing a simple acid-etched graphene oxide (d-GO) modification to address the high vanadium ion permeability as well as improve the stability of the membrane. The d-GO nanosheets, embedded within the perfluorosulfonic acid (PFSA) matrix, effectively suppress vanadium ion permeation by creating tortuous ion transport pathways, while promoting proton conductivity due to their hydrophilic nature. The membrane's unique sandwich structure, consisting of d-GO-modified PFSA as outer layers and a porous polytetrafluoroethylene (PTFE) core for mechanical reinforcement, ensures both ion selectivity and membrane stability. With the introduction of d-GO nanosheets and PTFE layer, the hybrid membrane shows a superior ion selectivity, excellent mechanical strength, and chemical stability in long-term cycling performance. Accordingly, electrochemical performance tests demonstrate that the hybrid membrane delivers a significantly improve compared to PFSA membranes [1]. This work provides a promising approach for advancing VRFB technology, offering both enhanced ion selectivity and operational stability. The findings can be extended to other fields where high ion selectivity and membrane stability are required, offering potential improvements in energy storage technologies.

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High energy-absorption structures bio-inspired from *Zoroaster Carinatus Philippinensis*

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Structural lightweighting means to minimize weight through optimized design, material selection, and manufacturing techniques, while prioritizing the functionality and safety of structures. The aim is to enhance energy efficiency and reduce energy consumption.[1] However, weight reducing often results in lower damage resistance.[2] Therefore, study on the key components which perform high loading resistance in structure systems becomes crucial. Biological structures, such as honeycombs and nacre shells, offer reliable design methods for light weight, high-energy absorption structures. Similarly, we noticed *Zoroaster Carinatus Philippinensis*, a type of sea stars which survive in deep-sea environments ranging from 200 to 6000 meters, relying on their high energy absorbing skeletons.[3] These skeletons are primarily composed of orderly arranged ossicle blocks which exhibit a foam-like morphology and a high porosity, performing an excellent weight reducing design. The mechanical testing on the unit structure of the blocks reveal that the oriented arrangement directs the anisotropy of the mechanical properties. Finite element simulations confirm that this performance is due to a combination of localized deformation and load redistribution mechanisms. In this work, a novel low-density, high-energy absorption porous skeletal structure model will be generated based on the mechanical properties of the microscopic architecture of this type of starfish.

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Dynamic Cu⁰/Cu^(I) Interface Promotes Acidic CO₂ Electoreduction

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Acidic CO₂ electroreduction with high carbon utilization efficiency encounters challenges with low C-C coupling ability. High alkali-cation concentrations, the main solution in reported works, will induce salt crystallization and block the CO₂ transport channel. Modulating Cu oxidation states is another strategy, whereas the Cu oxidation state cannot be maintained during CO₂RR. Thus, it is crucial to investigate a feasible strategy to boost C-C coupling and achieve high C₂₊ selectivity for acidic CO₂RR under low salt concentrations. In this work, we adopted an I₂-added strategy to construct dynamic Cu⁰/Cu^(I) interfaces during the acidic CO₂RR process, promote C-C coupling, and achieve a high FE_{C₂₊} of above 70% at 0.4 ~ 0.6 A cm⁻² under a low K⁺ concentration of 0.3 M. This is comparable to those acidic systems with almost ten times higher K⁺ concentrations, alleviating the salt crystallization on the gas transport channel. Based on the theoretical calculation and experimental characterizations, it can be concluded that the addition of I₂ in the electrolytes can induce the iodization of Cu into CuI, together with the reduction potentials, a redox loop of Cu → CuI → Cu exists during CO₂RR, and a dynamic Cu⁰/Cu^(I) interface generates. The special interface benefits the adsorption of *CO and the further C-C coupling process. This work shed light on the strategy for achieving high selectivity of C₂₊ products for acidic CO₂RR with low K⁺ concentrations.

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Lewis acid-induced reversible disproportionation of TEMPO enables aqueous aluminium radical batteries

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Multivalent metal ion batteries, including Al^{3+} , Zn^{2+} , or Mg^{2+} , use abundant elements in Earth's crust and provide much higher energy density than lithium-ion batteries (LIBs)[1]. Particularly, aluminium-ion batteries (AIBs) attract great attention because of their high theoretical volumetric capacity of 8056 mAh cm^{-3} and specific capacity of 2981 mAh g^{-1} when metal aluminium is used as the anode. Therefore, nitroxide radical polymers (NRPs) are the most successful polymer cathode materials in delivering a stable voltage output. NRPs have been implemented in LIBs, sodium-ion batteries (SIBs), zinc-ion batteries (ZIBs), and full polymer solid and redox flow batteries. However, 2, 2, 6, 6-tetramethylpiperidyl-1-oxy (TEMPO) derivatives and NRP materials are most used under neutral to basic conditions because they were found unstable in acidic conditions due to a disproportionation reaction that may lead to the potential degradation of nitroxide radicals. In this work[2], we explore the chemical and electrochemical reactions of TEMPO radicals in organic and aqueous solutions in the presence of a Lewis acid $\text{Al}(\text{OTf})_3$, one of the most used electrolytes for AAIBs. These findings lead to the first design of radical polymer aqueous AIBs that are fire-retarded and air-stable, delivering a stable voltage output of 1.25 V and a capacity of 110 mAh g^{-1} over 800 cycles with 0.028% loss per cycle. This work demonstrates the promise of using non-conjugated organic electroactive materials for cost-effective and safe AIBs that currently rely on conjugated organic molecules.

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Lithium ion migration in nano-confined water within 2D MoS₂ layers

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The migration of Li ions in confined water systems has significant implications for energy storage and transport technologies. Lithium ions in nano-confined water between two-dimensional MoS₂ sheets is influenced by the unique properties of both the confined water and the MoS₂ material itself. This study investigates the dynamics of Li ion migration in water confined within MoS₂ layers using first-principles simulations. We aim to understand the interplay between confinement effects and the ionic mobility of lithium within the water system. We employ density functional theory and ab initio molecular dynamics simulations to model the Li ion migration pathways under nano-confined water. The structural analysis of the confined water reveals unique hydrogen-bonding patterns, distinct from those in bulk ice or liquid water, which significantly influence Li ion diffusion mechanisms. We further explore the activation energy barriers associated with ion migration, providing a detailed comparison across different interlayer spacings. Our results demonstrate that reducing the confinement width enhances the interaction between the Li ion and the surrounding water molecules, leading to changes in the migration pathway and activation energies. Additionally, the MoS₂ layers influence the stability and coordination environment of Li ions, with potential applications in improving ionic conductivity in nanoconfined water systems. These findings offer valuable insights into the role of water and MoS₂ as a facilitator of ion transport, providing a potential avenue for optimizing materials for next-generation batteries and energy storage devices.

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ABSTRACTS

High-capacity and long-cycle $\text{MoS}_2@\text{MoO}_3$ nanocomposite anodes for lithium-ion batteries

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Abstract:

Molybdenum oxides and sulfides are both ideal materials for the ion battery with high theoretical capacity (over $600\text{mAh}\cdot\text{g}^{-1}$); however, their structural and chemical shortcomings limited the promotion and application in research of batteries. Core-sheath structure ($\text{MoS}_2@\text{MoO}_3$) combined some of the merits of the participants still faces many problems of fabrication (e.g., harsh conditions, high cost, etc.). In this study, core-sheath $\text{MoS}_2@\text{MoO}_3$ heterostructure (MSO) was synthesized successfully via a facile and simple in-situ method. Notably, as an anode in lithium-ion batteries, MSO delivered the highest specific capacity of 838.09 mAh/g at 0.05 A/g . Meanwhile, the capacity retained more than 80 % after 450 cycles. The outstanding electrochemical feature of MSO is ascribed to the rational sulfurated MoO_3 , showing a good anode candidate for LIBs.

One-dimensional moiré chains with partially-filled flat bands in two-dimensional twisted bilayer WSe₂

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Two-dimensional (2D) moiré systems based on twisted bilayer graphene and transition metal dichalcogenides provide a promising platform to investigate emergent phenomena driven by strong electron-electron interactions in partially-filled flat bands [1,2]. A natural question arises: is it possible to expand the 2D correlated moiré physics to one-dimensional (1D)? This requires selectively doping of 1D moiré chain embedded in the 2D moiré systems, which is an outstanding challenge in experiment and seems to be not within the grasp of today's technology. Therefore, an experimental demonstration of the 1D moiré chain with partially filled flat bands remains absent. Here we show that we can introduce 1D boundaries, separating two regions with different twist angles, in twisted bilayer WSe₂ by using scanning tunneling microscopy (STM), and demonstrate that the flat bands of moiré sites along the 1D boundaries can be selectively filled. The charge and discharge states of correlated moiré electrons in the 1D moiré chain can be directly imaged and manipulated by combining a back-gate voltage with the STM bias. Our results open the door for realizing new correlated electronic states of the 1D moiré chain in 2D systems [3].

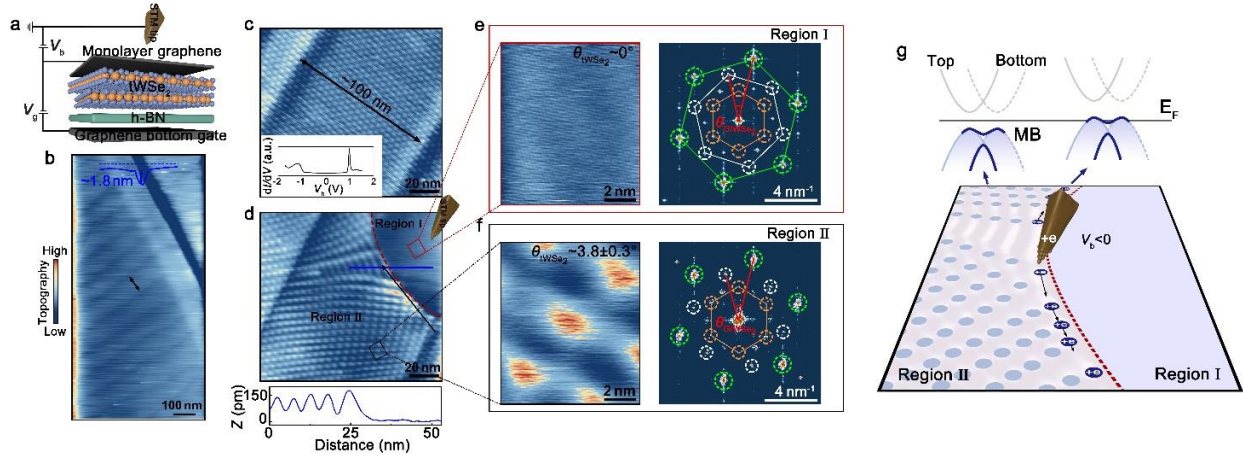


Fig 1. (a) Sketch of graphene/tWSe₂ heterostructure device used for STM study. (b) A large-scale STM topography image measured on the sample surface, revealing a quasi-1D superlattice with an approximate period of 100 nm. (c) A representative zoom-in STM topographic image reveals a moiré superlattice morphology with a period of about 4.4 nm. (d) STM topographic image after applying a tip voltage pulse. The moiré structure observed in the image exhibits two distinct regions. In region I, the moiré pattern completely vanishes. In region II, a conspicuous stretching of the moiré pattern is observed. (e,f) Atomic-resolved STM images and FFT images in the region I and region II, respectively. (g) Sketch of the tip-induced charging effect at the moiré sites along the 1D boundary. Under significant strain and local lattice rotations, the valence moiré band (MB) at the boundary moiré sites is tuned to approach the Fermi level. The STM tip serves as a local top gate, and when the applied bias voltage exceeds a certain threshold, the flat band crosses the Fermi level, leading to a charging response.

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Acidic CO₂-to-HCOOH Electrolysis with Industrial-level Current on Phase Engineered Tin Sulfide

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Acidic CO₂-to-HCOOH electrolysis represents a sustainable route for value-added CO₂ transformations. However, competing hydrogen evolution reaction (HER) in acid remains a great challenge for selective CO₂-to-HCOOH production, especially in industrial-level current densities. Main group metal sulfides derived S-doped metals have demonstrated enhanced CO₂-to-HCOOH selectivity in alkaline and neutral media by suppressing HER and tuning CO₂ reduction intermediates. Yet stabilizing these derived sulfur dopants on metal surfaces at large reductive potentials for industrial-level HCOOH production is still challenging in acidic medium. Herein, we report a phase-engineered tin sulfide pre-catalyst (π -SnS) with uniform rhombic dodecahedron structure that can derive metallic Sn catalyst with stabilized sulfur dopants for selective acidic CO₂-to-HCOOH electrolysis at industrial-level current densities. *In situ* characterizations and theoretical calculations reveal the π -SnS has stronger intrinsic Sn-S binding strength than the conventional phase, facilitating the stabilization of residual sulfur species in the Sn subsurface. These dopants effectively modulate the CO₂RR intermediates coverage in acidic medium by enhancing *OCHO intermediate adsorption and weakening *H binding. As a result, the derived catalyst (Sn(S)-H) demonstrates significantly high Faradaic efficiency (92.15 %) and carbon efficiency (36.43 %) to HCOOH at industrial current densities (up to -1 A cm^{-2}) in acidic medium.

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DFT study of high-entropy MOF applied in water splitting as electrocatalysts

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Metal-organic frameworks (MOFs) have emerged as promising materials for electrocatalysis for water splitting due to their high specific surface area, structural tunability, and stability [1]. However, notable challenges persist, including dependence on precious metals, susceptibility to dissolution in acidic environments at elevated potentials, and the necessity for enhanced intrinsic activity and stability, which requires careful consideration and resolution [2].

This work investigates the catalytic performance of various MOFs, with a particular focus on high-entropy materials, where the introduction of configurational entropy through elemental substitution enhances properties such as strength, decomposition resistance, and thermal stability. Using Density Functional Theory (DFT) calculations, we explore the structural and electronic modifications of UiO-66 as a representation of MOFs to improve their catalytic activity in water splitting. By substituting different metals for Zr in the UiO-66 framework to increase the entropy of the material, we demonstrate significant and impressive improvements in OER overpotentials, particularly in materials such as Ag-UiO-66 and Tc-UiO-66. These enhancements are attributed to electronic interactions and optimized electron transfer processes. The insights gained from this theoretical study provide valuable guidelines for designing next-generation MOF-based electrocatalysts for sustainable energy applications, which paves the way to explore trimetallic MOF systems for further catalytic improvements.

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Ab Initio Investigation of Layered MoS₂ Electrodes for Aqueous Zinc Batteries

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Aqueous zinc batteries present a niche and growing field of secondary batteries that are stable in aqueous environments. With high theoretical volumetric capacity and low cost, zinc batteries promise useable grid scale renewable energy storage. Current zinc batteries suffer from inferior electrochemical and kinetic performance due to poor accommodation of zinc within the electrode. Engineered transition metal dichalcogenides (TMDs), with their tunable interlayer spacings, are a promising class of materials for the electrodes to address these limitations, offering potential for fast atomic transport and effective intercalation. The impact of water is a recent focus

Here we investigate in detail the atomic scale mechanism of aqueous zinc intercalation in a prototypical layer-expanded TMD, MoS₂. Using systematic first principles density functional theory simulations, we show that the presence of water molecules within bulk unmodified MoS₂ decreases stability and diffusion kinetics of intercalated zinc.

Optimisation of interlayer distances improves the kinetics in all cases. 1T-MoS₂ retains a stable calculated voltage of 0.8 V, showing suitability as the anode material, while 2H-MoS₂ has poor stability above zinc concentrations of 0.03 per MoS₂ formula unit. 1T-MoS₂ is thermodynamically favourable above zinc concentrations of 0.25 zinc per MoS₂ formula unit at all engineered interlayer distances, with a specific capacity of 232 mAh g⁻¹. The key findings of the study advance the understanding of the trade-off between electrochemical capacity and kinetics, thus highlighting an approach to improved anodic performance of MoS₂ for aqueous zinc batteries. The effect of infiltrated water on zinc intercalation is key for achieving this understanding and is essential for future of aqueous zinc battery technology.

Effects of the modification of functional surface oxygen-based groups on molybdenum disulfide moisture electricity generators

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Moisture-electricity generators (MEGs) are emerging as promising sustainable power sources, capable of addressing the energy crisis by harvesting low-level energy from ambient moisture without requiring mechanical, thermal, or solar input [1]. However, it remains a challenge to understand the underlying process of electricity generation of MEGs. We present an asymmetrically structured generator using 2D molybdenum disulfide as the middle functional layer. The correlations between the various oxygen functional groups elements and the moisture-electric performance is investigated.

Experimental results indicate that modifying molybdenum disulfide with varying ratios of carboxyl functional groups significantly enhances electricity generation. This improvement is primarily attributed to the increased water absorption capacity of the functional layer and the accelerated hydrolysis process facilitated by the carboxyl groups. The carboxyl-modified molybdenum disulfide nanosheet-based MEGs achieved a voltage exceeding $550 \text{ mV} \cdot \text{cm}^{-2}$ and a current density of $10.1 \mu\text{A} \cdot \text{cm}^{-2}$ at 85% relative humidity. Additionally, higher voltages can be easily obtained through series or parallel connections, enabling the device to power small-scale appliances. This study underscores the crucial role of carboxyl groups in the hydro-electrical conversion process of 2D molybdenum disulfide and provides valuable insights for developing high-performance MEGs.

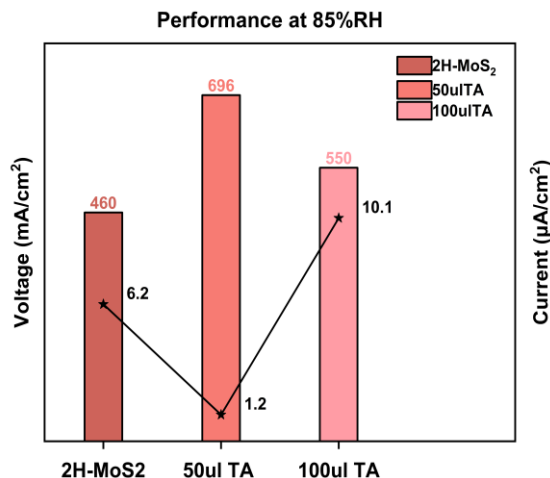


Figure 3 Molybdenum Disulfide MEG E-performance at 85%RH

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Structural evolution of copper-silver alloy using machine learning accelerated molecular dynamics

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Understanding the structural evolution of materials during operation is central to advancing materials science. In this study, we used copper-silver alloy as example, employed machine learning accelerated molecular dynamics (ML-MD) to simulate its structural evolution in long-period. Copper-silver “alloy” is widely utilized in electrochemical CO₂ reduction, with ability of enhancing activities and shifting selectivity. However, thermodynamic phase diagrams show that Cu and Ag are difficult to alloy at room temperature, introducing uncertainties in catalyst surface models and limiting deeper mechanistic studies. We addressed this challenge by using ML-MD models trained on density functional theory (DFT) data through active learning. These models achieve high accuracy while remaining computationally efficient. Our results reveal that annealing induces the formation of a pure silver layer on the surface within nanoseconds, driven by the lower surface energy of silver. In the bulk, phase separation between copper and silver occurs as the simulation scale increases. This work provides new insights into the structural evolution of copper-silver alloys from a computational perspective, which would contribute to the design of future catalytic materials.

2D Ultrathin Iron Doped Bismuth Oxychloride with Oxygen Vacancy for Enhanced Sonodynamic Therapy

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In this work, ultrathin Fe-doped bismuth oxychloride (BiOCl) nanosheets (BOC-Fe NSs) with oxygen vacancy and bovine serum albumin (BSA) coating on surface are designed as piezoelectric sonosensitizers for enhanced SDT (Figure 1A, 1B). The oxygen vacancy of BOC-Fe NSs provides electron trapping sites and promotes the separation of e^-h^+ from the band structure, enhancing the ROS production under the ultrasonic waves (Figure 1C). The piezoelectric BOC-Fe NSs creates a built-in field and the bending bands, further accelerating the ROS generation with ultrasound irradiation. Furthermore, BOC-Fe NSs could induce ROS generation by a Fenton reaction catalysed by Fe ion. The as-prepared BOC-Fe NSs efficiently inhibited breast cancer cell growth in in-vitro test. The successful development of BOC-Fe NSs provides a new nano-sonosensitiser option for enhanced SDT for cancer therapy.

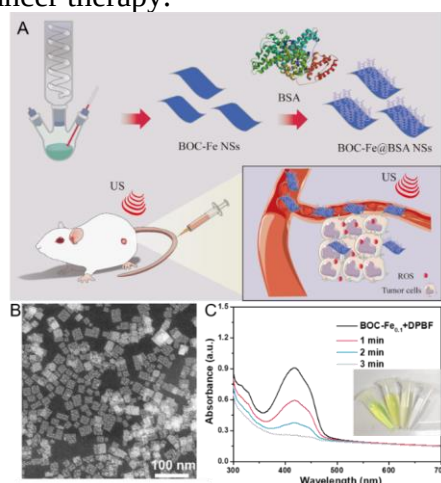


Figure 1. The preparation of BOC-Fe NSs for enhanced SDT. (A) The preparation procedure of BOC-Fe NSs for SDT. (B) STEM images in dark field of BOC-Fe NSs. (C) ROS production performance of BOC-Fe NSs using the DPBF probe.

Aqueous Zinc–Iodine Pouch Cells with Long Cycling Life and Low Self-Discharge

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Aqueous zinc batteries are promising candidates for large-scale energy storage due to their cost-effectiveness and safety. However, their widespread application has been hindered by the lack of affordable electrolytes capable of stabilizing both the cathode and anode. In this work, we present an innovative approach to improving zinc-iodine batteries by incorporating a trace amount of an imidazolium-based additive into a cost-effective zinc sulfate electrolyte. This additive bonds with polyiodides, significantly enhancing anti-self-discharge properties and cycling stability. Furthermore, additive aggregation at the cathode improves I₂ conversion kinetics, resulting in better rate capacity, while it also enhances the reversibility of zinc deposition at the anode.

Our zinc-iodine pouch cell demonstrated impressive industrial-level performance, with a Coulombic efficiency of ~99.98% at 0.4C, a low self-discharge rate with only 11.7% capacity loss per month, and excellent long-term cycling stability, retaining 88.3% of its initial capacity after 5000 cycles at a zinc depth-of-discharge of 68.3%. Additionally, the cell achieved rapid charging at ~6.7C with high active-mass loading (>15 mg cm⁻²). Notably, the self-discharge performance exceeds that of commercial nickel-metal hydride batteries and rivals commercial lead-acid batteries, while its lifespan is over 10 times longer than previously reported zinc-iodine systems. Moreover, the fast-charging capability surpasses that of commercial lithium-ion batteries, making this a highly competitive solution for future energy storage systems.

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van der Waals integrated dielectric for future two dimensional electronics

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Two-dimensional systems hold great potential for developing next-generation electronic devices to extend the Moore law. To achieve this, one significant challenge is to improve the interface quality between semiconductors and the dielectrics, which are difficult to achieve by conventional deposition technology. In this poster, we demonstrate two kinds of novel dielectric (SrTiO₃^[1] and Diamane^[2]), which can be integrated with two-dimensional systems (hydrogenated diamond and two-dimensional transition metal dichalcogenide) via van der Waals forces, thus enhancing the device performance.

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A Selective Salt Crystallization and Deposition Solar Evaporator with a Parallel Water Supply Strategy for Long-term and Highly Efficient Solar Steam Generation

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Interfacial solar evaporation presents a green and sustainable approach to alleviate clean water shortage through solar-driven desalination. Over the past decade, significant research efforts have focused on increasing evaporation rates, yielding notable advancements [1]. However, the faster evaporation rates may lead to salt crystallization and accumulation on evaporation surfaces which cause considerable heat loss, substantially decreased light absorption and evaporation rates, posing a significant challenge for long-term practical application [2, 3]. To tackle this challenge, this study introduces an innovative photothermal evaporator with a parallel water supply strategy for long-term and highly efficient solar steam generation. In contrast to conventional single-water path systems that often result in salt accumulation at the furthest parts of water supply paths, the introduction of a secondary parallel water path completely re-configures the ion diffusion and distribution within the system, preventing salt crystallization and accumulation on both evaporation surfaces and water paths. Consequently, it effectively eliminates the adverse impact of salt crystallization on evaporation performance and allows for easy salt collection. This approach holds practical significance for the design and application of solar evaporators for long-term operation.

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Lattice-water-assisted Oxygen Exchange for High-performance Proton Exchange Membrane Water Electrolyzers

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A trade-off between activity and stability of oxygen evolution reaction (OER) catalysts in proton exchange membrane water electrolyzer (PEMWE) is challenging. Crystalline IrO₂ displays good stability but exhibits poor activity; amorphous IrO_x exhibits outstanding activity while sacrificing stability.^[1-3] Here, we combine advantage of these two materials via a lattice water-incorporated iridium oxide (IrO_x·nH₂O) that has short-range ordered structure of hollandite-like framework. We confirm that IrO_x·nH₂O exhibits boosted activity and ultrahigh stability of > 5,700 hours (~8 months) with a record-high stability number of 1.9×10^7 n_{oxygen} nIr⁻¹. We evidence lattice water is active oxygen species in sustainable and rapid oxygen exchange. The lattice-water-assisted modified OER mechanism contributes to improved activity and concurrent stability with no apparent structural degradation, which is different from the conventional adsorbate evolution mechanism (AEM) and lattice oxygen mechanism (LOM). We demonstrate that a high-performance PEMWE with IrO_x·nH₂O as anode electrocatalyst delivers a cell voltage of 1.77 V at 1 A cm⁻² for 600 h (60 °C).^[4]

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Direct observation of photoinduced carrier blocking in mixed-dimensional 2D/3D perovskites and the origin

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Mixed-dimensional 2D/3D halide perovskite solar cells promise high stability but practically deliver poor power conversion efficiency, and the 2D HP component has been held as the culprit because its intrinsic downsides (ill charge conductivity, wider bandgap, and strong exciton binding) were intuitively deemed to hinder carrier transport. Herein, we show that the 2D HP fragments, in fact, allow free migration of carriers in darkness but only block the carrier transport under illumination. While surely limiting the photovoltaic performance, such photoinduced carrier blocking effect is unexplainable by the traditional understanding above but is found to stem from the trap-filling-enhanced built-in potential of the 2D/3D HP interface. By parsing the depth-profile nanoscopic phase arrangement of the mixed-dimensional 2D/3D HP film for solar cells and revealing a photoinduced potential barrier up to several hundred meV, we further elucidate how the photoinduced carrier blocking mechanism jeopardizes the short-circuit current and fill factor.

Photocatalytic Upcycling of Plastic Waste to Hydrogen Fuel and Commodity Chemicals

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An estimated 8 billion tonnes of plastic have been manufactured, most (ca. 80%) however end up in landfills and aquatic systems,^[1] posing a serious threat to the ecological environment and a waste of carbon resources. Therefore, there is an urgent need to develop sustainable recycling methods to mitigate plastic pollution and recover value from waste.

Solar-driven photocatalysis is a sustainable technology that utilizes solar photon-induced charge carriers to carry out chemical reactions under ambient conditions.^[2] It offers a practically promising approach to re-/upcycle plastic waste for addressing contemporary energy and environmental challenges. Photocatalytic upcycling of plastic waste harnesses renewable solar energy to generate clean fuels (such as hydrogen) and valuable chemicals *via* valorization of plastic waste.^[1] The process mitigates plastic waste and fossil energy inputs, addressing environmental issues of waste plastic accumulation and greenhouse gas emissions derived from fossil fuels. Additionally, it can be safely operated under mild conditions and has practical potential to be upgraded to flow processing and up-scale reaction systems. The key to the implementation of this technology depends on efficient photocatalysts and appropriate reaction systems.

Our research focuses on the development of atomically engineered photocatalysts.^[1,2] By introducing /regulating atomic-level active sites (e.g., atomic defects and single atoms) in photocatalysts, the charge separation/migration and surface catalytic reactions can be significantly boosted. Combined with tailored batch /flow reactors, we achieved efficient and selective conversion of plastic waste into hydrogen and organic acids under ambient conditions. Our work offers a sustainable and attractive method to generate value-added products from waste, contributing to the circular economy.

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Hidden Acidification Challenges in Electrochemical Ocean Decarbonization

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Seawater, the largest carbon sink, absorbs atmospheric carbon dioxide (CO₂) to balance global carbon cycle. Rising CO₂ emissions lead to ocean acidification [1,2]. The average pH of ocean surface decreases from ~8.15 to ~8.05 between 1950 and 2020, threatening marine organisms and the ocean's carbon absorption capacity

Electricity-powered pH swing technology offers a dual benefit: it removes carbon from the ocean and mitigates ocean acidification. The sustainability of this technology is now challenged by 1) the complexity of seawater ions; 2) charge and efficiency balance; and 3) further ocean acidification. Here we report a comprehensive analysis of electrochemical direct ocean capture (DOC) under thermodynamic equilibrium, considering products, charges, and ultimate effects on ocean acidification. We find a nearly 100% carbon removal efficiency via acidification (pH 4.2) or alkalization (pH 8.6), with a minimum theoretical charge of 244 coulombs per liter (C/L). Compared to the initial oceanic pH of ~8.1, the results (DpH_{acid}=3.9, DpH_{alka}=0.5) ($\text{DH}^+ = 7.5 \times 10^{-5}$, $\text{DOH}^- = 3.0 \times 10^{-6}$) revealed an asynchronous nature of electrochemical strategies. Therefore, we analyzed the mixture of acidic and basic seawater after the operation cannot be neutralized (pH < 6.5). As a result, our study – in light of non-equivalent variation of pH – revealed the water neutralization as the key challenge ahead.

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