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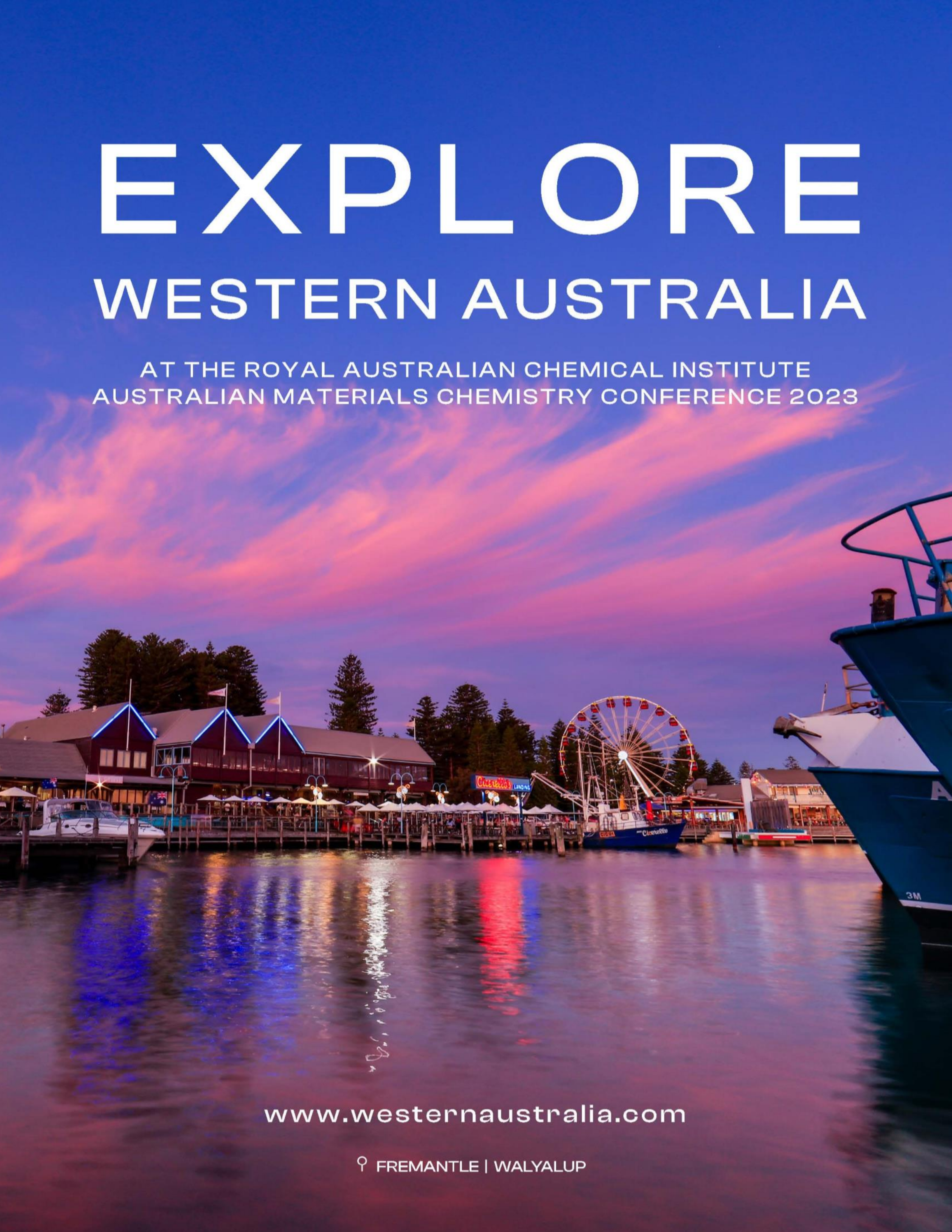

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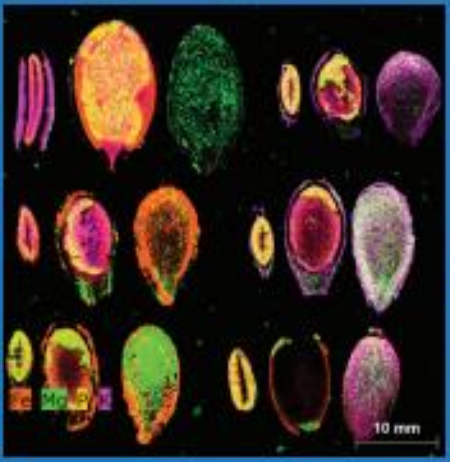

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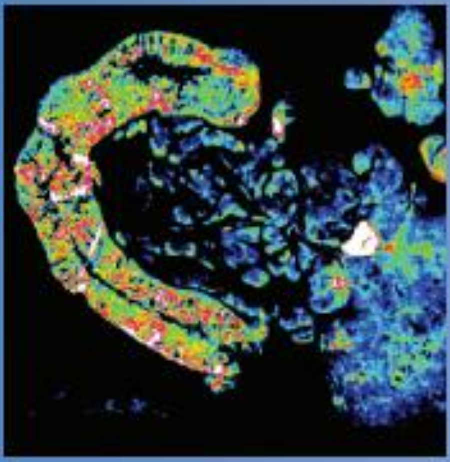

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Organised in partnership with The Royal Australian Chemical Institute (RACI), the AMCC23 offers the materials chemistry community a highly visible platform to showcase their latest and new research. The conference will bring together experts from all subjects of materials chemistry to create a forum for fundamental and applied science.

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Thank you for being a part of this great event.

Guohua Jia

Associate Prof. Guohua Jia
Conference Chair
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Plenary speakers

Prof. Debra Bernhardt

University of Queensland

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

Plenary speakers

Prof. Dmitri Golberg

Queensland University of Technology

Prof. Dmitri Golberg has a wide background and strong command in the synthesis, structural analysis, and physical property measurements of diverse inorganic nanotubes, nanowires, graphene-like nanosheets, nanoribbons and nanobelts. After getting PhD and 10 years research career at the Bardin Research Institute in Moscow, in 1995 he joined the National Institute for Materials Science (NIMS) in Tsukuba, Japan, and became one of the first researchers in the world to launch pioneering studies on boron nitride nanotubes. Since then he became a world-recognized expert in this field and published more than 200 papers solely on the nano-BN topic. In 2016 Dmitri won an Australian Laureate Fellowship, and in 2017 joined QUT after more than 20 years of Nanotube Group Leadership at NIMS. During his career Dmitri secured the prestigious Tsukuba Prize (2005), Thomson Reuters Research Front Award (2012), Seto Prize by Japan Microscopy Society (2016), and NIMS President Award (2017). He was also nominated as a Highly Cited Researcher in Materials Science by Thomson Reuters during consecutive years 2014-2021.

Plenary speakers

Prof. Baohua Jia

RMIT University

Baohua Jia joined RMIT in 2022 as a full professor and Australian Research Council Future Fellow (Level 3) in School of Science. She is the inaugural Director of Australian Centre for Atomaterials and Nanomanufacturing (ACAN). Before joining RMIT Baohua Jia was a full Professor, Founding Director of Centre for Translational Atomaterials and Research Leader at Swinburne University of Technology. She received her BSc and MSc degrees from Nankai University, China. She was awarded a PhD from Swinburne University of Technology, Australia. Professor Jia is an elected Fellow of Optica (previously known as Optical Society of America (OSA)) and an elected Fellow of Institute of Materials, Minerals and Mining (IoM3). Since 2019, Professor Jia has been serving as the Australian Research Council College of Expert.

Prof. Jia's research focuses on the fundamental light and nanomaterial interaction. In particular her work on laser manipulation of two-dimensional materials has led to the design and fabrication of functional nanostructures and nanomaterials for effective harnessing and storage of clean energy from sunlight, purifying water and air for clean environment and imaging and spectroscopy and nanofabrication using ultrafast laser towards fast-speed all-optical communications and intelligent manufacturing.

Plenary speakers

Prof. Douglas Macfarlane

Monash University

Professor Doug MacFarlane is a Sir John Monash Distinguished Professor and was recently an Australian Laureate Fellow at Monash University's School of Chemistry. His interests cover a broad range of materials chemistry and electrochemistry for renewable energy generation and storage. He has published more than 800 papers and 30 patents and these have been cited more than 75,000 times (h-index 132). He has been one of the Clarivate Highly Cited authors since 2020. He was the Australian Academy of Science's Craig Medalist 2018 and winner of the Victoria Prize for Science and Innovation 2018. Professor MacFarlane was elected to the Australian Academy of Science in 2007 and the Academy of Technological Sciences and Engineering in 2009. He recently founded a spin out company Jupiter Ionics to scale up the ammonia production technology his group has developed. Doug is a member of Editorial Advisory Boards of Chem Commun, Green Chem, ChemSusChem, and Sustainable Energy and Fuels.

ABSTRACT FORM PLENARY LECTURES (PL)

PL01	**Prof.**	**Debra Bernhardt**	**The University of Queensland**
PL02	**Prof.**	**Dmitri Golberg**	**Queensland University of Technology**
PL03	**Prof.**	**Baohua Jia**	**RMIT University**
PL04	**Prof.**	**Douglas Macfarlane**	**Monash University**

PL01 Modelling materials at the atomic and molecular level: Application to batteries and supercapacitors

Debra J. Searles (Bernhardt),[1,2]* Sobin Alosious, Ardeshir Baktash,[1,3] Baris Demir,[1] Tanika Duivenvoorden,[1,2] Stephen Sanderson,[1] Shern R. Tee,[1,4] Mingchao Wang,[1] Qinghong Yuan[1,5]

[1] Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Queensland 4072, Australia
[2] School of Chemistry and Molecular Biosciences, The University of Queensland, Queensland 4072, Australia
[3] School of Chemical Engineering, The University of Queensland, Queensland 4072, Australia
[4] School of Environment and Science, Griffith University, Nathan, QLD, 4111, Australia
[5] School of Physics and Electronic Science, East China Normal University, 500 Dongchuan Road, Shanghai, 200241, People's Republic of China

**Email: d.bernhardt@uq.edu.au*

Enhanced computational methods and greatly increase compute power are enabling more complex materials and systems to be modelled for longer times. However, the results obtained are only as good as the model and the analysis. In this talk we will demonstrate this through presentation of results of studies on supercapacitors and batteries.[1-4.] Supercapacitors are known for their high power density, but low energy density, so new materials are being proposed that can increase the energy density without loss in the power density. In the case of batteries, finding highly conductive, safe electrolytes that interface well with the electrode is key. Simulations have assisted in improving these energy storage systems, but this has required improvements in the computational methods to provide more accurate results and, also consideration of the qualitative predictions on the systems. We will present some results from our research that illustrate this.

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PL02 Boron nitride nanotubes and nanosheets: synthesis, properties and applications

Dmitri Golberg, [1,2]*

[1] Centre for Materials Science and School of Chemistry and Physics, Queensland University of Technology (QUT), 2 George, Brisbane, QLD 4000, Australia
[2] Research Centre for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS) Namiki 1, Tsukuba, Ibaraki 305, Japan

**Email: dmitry.golberg.@qut.edu.au*

Synthetic routes and electromechanical properties of pristine and carbon-doped BN nanotubes[1] 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). Elastic modulus, tensile strength,[2,3] fracture toughness, conductivity of 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 utilised 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*., CO_2 hydrogenation, CO oxidation *etc*., hydrogen accumulation,[4] 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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PL03 Atomaterials for sustainability

Baohua Jia [1]*

[1] *School of Science, RMIT University, 124 La Trobe Street, Melbourne 3000, Australia*

**Email: baohua.jia@rmit.edu.au*

“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. These materials play critical role in improving energy efficiency and providing innovative sustainable solutions for our society.

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PL04 Ionic materials for electrochemical generation of ammonia as an energy carrier

Douglas R. MacFarlane [1]*, Hoang-Long Du [1] and Alexandr N. Simonov [1]

[1] School of Chemistry, Monash University, Clayton, Victoria 3800
**Email: douglas.macfarlane@monash.edu*

Green ammonia has become widely recognized in recent years as a potential component of the future global energy economy. Produced from renewables, N_2 and water, ammonia can be viewed as an energy carrier that can be used as fuel in combustion engines, turbines and even co-firing along with other fuels. Of course, green ammonia also has an important role in displacing fossil fuel produced ammonia in the fertilizer and chemicals supply chains. In our recent work we have demonstrated a Li-mediated electrochemical process that produces NH_3 at high rates with faradaic efficiencies approaching 100%.[1, 2] A variety of proton carriers can be productive in this role including the well-known ethanol and the phosphonium ylide, these studies providing some indication of the key properties that such a proton carrier must possess. These include (i) sufficient mobility in the electrolyte medium such that mass transport is not limiting, (ii) sufficient electrochemical stability such that the proton carrier is not reactive on the electrodes, in either its protonated or deprotonated form and (iii) sufficient (very weak) acidity to protonate the Li_3N, while at the same time not overpopulating the cathode with absorbed H atoms such that H_2 production becomes a significant parallel reaction. It is clearly highly desirable to understand the interplay between these key properties in a more detailed fashion in order to optimise the outcomes of this process and also to understand how the optimum properties of the proton carrier may be impacted by changes in other electrolyte components including the solvent and the lithium salt.

In this work we have explored a range of proton carriers from the alcohol family in this process alongside the phosphonium type of carrier and ammonia itself, investigating their impact on yield and selectivity. Some aspects of this study have been published recently.[3]

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ABSTRACT FORM KEYNOTE LECTURE(KL)

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KL01 Potential dependent dynamics of ionic liquids at graphite electrodes revealed by atomic force microscope videos

Rob Atkin,[1,*] Hua Li,[1] Jianan Wang[1]
[1]School of Molecular Sciences, The University of Western Australia, Perth, Western Australia, Australia
* Email: rob.atkin@uwa.edu.au

The nanostructure of ionic liquids above electrodes has not previously been studied experimentally in real time. This means the dynamics of ionic liquid processes at interfaces are relatively poorly understood, and the mechanisms of, for example, charging and discharging at electrodes, lubrication and heterogenous catalysis are unclear. The aim of this work is to probe the structure and dynamics of ionic liquids at electrodes and the effect of variation in the electrode potential. Video-rate atomic force microscopy is used to study the near-surface nanostructure of the ionic liquids ethylammonium nitrate (EAN), 1-butyl-3-methylimidazolium dicyanamide (BMIM DCA) and 1-hexyl-3-methylimidazolium dicyanamide (HMIM DCA) at graphite electrodes as a function of potential. AFM videos reveal slow moving near-surface nanostructures that migrate, merge and rupture over time, as shown in the snapshots for EAN in Figure 1. Disk-like features 5 – 10 nm in diameter and ~1 nm in height form on top of the Stern layer at all potentials. The nanostructure diffusion coefficient varies with the ionic liquid type and surface potential and is ~ 8 orders of magnitude lower than the diffusion coefficients for individual ions in the bulk. Ionic liquid nanostructures at electrodes are often described as “near-surface liquid layers” but this work shows this terminology is misleading. The near-surface liquid nanostructure is much richer than simple layers and is better conceptualized aggregates slowly migrating over the Stern layer.

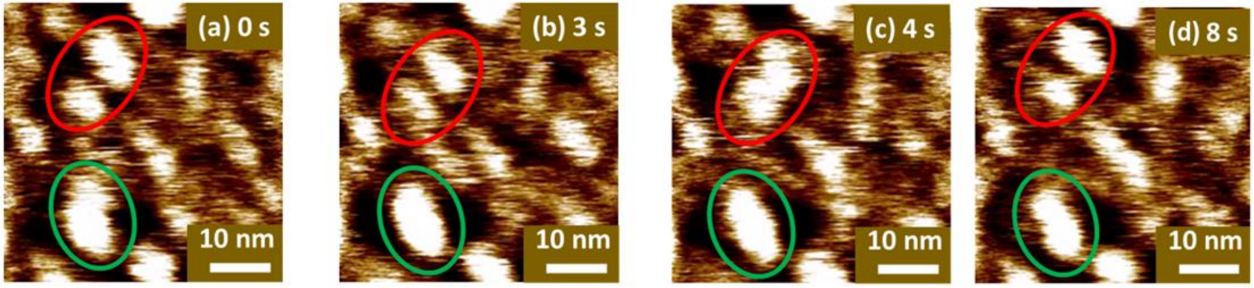

Figure 1. Frames from AFM topographic videos for pure EAN on graphite at OCP. The time (s) is shown in the top right of the frames. The feature circled in green moves extremely slowly and was visible for 32 s. The nanofeatures within the red circle merge at 4 s and then rupture at 8 s.

KL02 Zero-emission thermoelectric power generation and coolers for carbon neutrality

Zhi-Gang Chen[a,b]
[a]School of Chemistry and Physics, Queensland University of Technology, Brisbane, Queensland 4001, Australia
[b]ARC Research Hub in Zero-emission Power Generation for Carbon Neutrality (ZeroPC), Queensland University of Technology, Brisbane, Queensland 4001, Australia

* Email: zhigang.chen@qut.edu.au

Climate change caused by the continuous accumulation of greenhouse gas is an imminent threat to mankind and biodiversity. Already a dry land with vulnerable biodiversity, Australia will be hard hit by climate change as evidenced by the recent natural disasters with much increased frequency and intensity. To stop climate change, we need significantly reduce carbon dioxide (CO_2) to net-zero emissions. In this topic, we timely highlight the latest progress on the up-to-the-date thermoelectric devices with their unique designs and compelling thermoelectric efficiency for harvesting renewable electricity from environment, which will reduce our dependence on carbon-based energy sources. Here, we carefully summarize the structure-related principles and factors that determine the performance of thermoelectric devices and propose strategies for improving their utilities. Besides, we focus on the timeliest designs for inorganic-based devices, organic-based devices, and hybrid-based devices targeting for both power generation for zero-emission. In the end, we point out the current challenges, controversies, and prospects of thermoelectric devices.

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KL03 Molecular carbons with different topologies and size

Chunyan Chi[1]*

[1]Department of Chemistry, National University of Singapore, Singapore
**Email: chmcc@nus.edu.sg*

Carbon-based nanostructures have shown revolutionary influence in the area of chemistry, physics and materials science. Recent efforts have been focused on novel topological structures of sp^2-carbons such as carbon nanohoops, nanobelts, molecular cages, and open-shell nanographenes, which provoked new chemistry and materials. However, synthesis of this kind of molecules is extremely challenging mainly due to strain or intrinsic high reactivity. Another issue is that most of these carbon nanostructures have a localized aromatic character; that means, the π-electrons are not globally delocalized along the backbone, which limits their optical and electronic properties and applications. Herein, the synthesis of a series of novel pi-structure with different topologies will be introduced, and their physical properties, aromaticity and diradical character will be discussed.[1-7]

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KL04 Ultrathin nanosheets: sustainable synthesis and biomedical applications

Zi Sophia Gu[1]*

[1] School of Chemical Engineering, University of New South Wales, Sydney, NSW 2051, Australia
[2] Australian Centre for NanoMedicine, University of New South Wales, Sydney, NSW 2051, Australia
[3] UNSW RNA Institute, University of New South Wales, Sydney, NSW 2051, Australia
**Email: zi.gu1@unsw.edu.au*

Nanotechnology has emerged as a promising approach for precision treatment of life-threatening diseases.[1] Two-dimensional nanoparticle-based therapeutic agents have been developed for safe and efficient treatment of diseases. Nanomaterial innovation play a key role in driving progress of the field.[2] In this talk, I will present our recent work on the sustainable synthesis of monolayer layered double hydroxide (LDH) nanosheets and their biomedical applications in drug delivery, catalytic cancer therapy, and theranostic nanomedicine. We synthesise ultrathin LDH nanosheets via a polymer-assisted bottom-up method that was recently developed in our laboratory.[3,4] By using this method, a library of LDH nanosheets have been synthesised, which contain various functional metal cations and ions. The ferrous-containing LDH nanosheets demonstrated high catalytic activity to disproportionate hydrogen peroxide in tumours and in-situ generated hydroxyl radicals efficiently to kill tumour cells.[3] The production of hydroxyl radicals can be enhanced by cascade catalytic reactions triggered by photocatalysis.[5] The nanosheet also generated oxygen bubbles and promoted the long-distance and directional movement toward the tumour microenvironment, thus achieving targeted delivery of therapeutic agents.[6] By delivering a model drug doxorubicin, we demonstrated a ultra-high drug loading system by using our ultrathin nanosheets.[7] The nanosheets can also be used as a molecular imaging diagnostic probe for tumour detection and theranostic nanomedicine.[8]

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KL05 Ultrastrong nanotwinned titanium alloys through additive manufacturing

Aijun Huang[1*]

[1] *Department of Materials Science and Engineering, Monash University, VIC 3800, Australia.*
**Email: aijun.huang@monash.edu*

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

KL06 Understanding the epitaxial growth of graphene on 3C-SiC using a Ni/Cu alloy

Francesca Iacopi, [1,2]*

[1] University of Technology Sydney, Faculty of Engineering and IT
[2] ARC Centre of Excellence in Transformative Meta-Optical Systems (TMOS)
**Email: francesca.iacopi@uts.edu.au*

The harnessing of graphene's properties on a silicon platform could deliver a broad range of novel miniaturized and reconfigurable functionalities. In addition, some key functionalities for MEMS/NEMS, nano-optics and metasurfaces can be uniquely unlocked by the combination of graphene with silicon carbide [1, 2, 3].

Over the last decade, we have developed an epitaxial graphene on silicon carbide on silicon technology that inherently delivers both capabilities. This platform allows to fabricate any complex graphene flat or 3D nanopattern in a site – selective fashion, ie without etching of the graphene, at the wafer -scale and with sufficient adhesion for integration [1, 4].

Obtaining a consistent epitaxial graphene coverage over the very defective 3C-SiC on silicon template has been a very challenging task that we have overcome with the use of a Ni/Cu metal alloy catalyst [5]. We have recently been able to confirm our hypotheses regarding the detailed mechanism of this approach with the help of in-situ neutron reflectometry performed at the ANSTO facilities. We will review the learnings from the development of this technology and some of its most promising applications [6, 7, 8].

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KL07 High throughput correlative electrochemistry-microscopy analysis on complex electrodes

Minkyung Kang* and Gunani Deekirike Jayamaha Mudalige

School of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia
**Email: Minkyung.kang@sydney.edu.au*

Conventional electrodes and electrocatalysts are known to possess complex elements that impact their overall electrochemical activity. These elements range from defects and crystal orientation on the electrode surface to layers and composites with other electrode components such as binders. It is, therefore, vital to identify how these individual elements alter the electrochemical activity of the electrode. Scanning electrochemical cell microscopy (SECCM) is a powerful tool that has been developed for investigating the electrochemical properties of these complex structures.[1] SECCM is a versatile and robust electrochemical imaging technique that allows for the direct correlation of structure and activity at the nanoscale. By using a mobile droplet cell to confine the unit of interest in a small volume, it has been utilised to visualize and investigate the electrochemical activity at interfaces with high spatiotemporal resolution.

In this study, voltammetric SECCM together with correlative microstructure analysis was employed to screen complex electrode surfaces with high throughput. The analysis revealed that dislocation density and crystal orientation play an essential role in electrochemical CO_2 conversion on structurally heterogeneous polycrystals such as polycrystalline Au and Cu. The SECCM data has been analysed with identical location electron backscatter diffraction (EBSD) obtained from 2 to 60 individual grains containing 700 to 2500 voltammetric SECCM measurements, respectively.[2,3] The similar strategy has been deployed to study as-cast ZnAl alloy, which is utilised in many applications in multiple sectors ranging from cathodic protection of steel to battery electrodes. As-cast ZnAl alloy presents complex surface features, such as three different phases (i.e., α, β, and η), containing various composition ratios of Al/Zn ranging from 1 to 40 %, as well as a fine lamellar structure that forms during the phase transition when rapidly cooling during alloy casting. The SECCM scan has covered a range of microstructural features with 651 voltammetric measurements in six distinctive areas on the ZnAl alloy surface. An identical location energy dispersive spectroscopy (EDS) map has revealed that both heterogeneous electrochemical reduction processes and various early metal dissolution rates are attributable to the alloy structure, specifically related to α-phase ZnAl alloy. In conclusion, high throughput electrochemical screening via SECCM in conjunction with correlative microstructure analysis unambiguously identify that heterogeneity in structure-composition significantly impacts local electrochemical activity on a complex electrode surface, ultimately providing insights for the rational design of electro-materials.

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KL08 Self-propelled biocatalytic nano/microswimmers for cancer diagnosis and therapy

Kang Liang*

School of Chemical Engineering, Graduate School of Biomedical Engineering, Australian Centre for Nanomedicine, The University of New South Wales, Sydney NSW 2052
**Email: kang.liang@unsw.edu.au*

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

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

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KL09 EXPLORING FERROELECTRIC DOMAIN SWITCHING BEHAVIOURS USING IN-SITU STRESSING AND BIASING TRANSMISSION ELECTRON MICROSCOPY

Xiaozhou Liao[1]*

[1] *School of Aerospace, Mechanical and Mechatronic Engineering,*
The University of Sydney, Australia.

**Email: xiaozhou.liao@sydney.edu.au*

Ferroelectric materials exhibit spontaneous polarization due to the displacement of ions, resulting in an internal electric field that points towards a specific direction. These materials are composed of regions known as ferroelectric domains, each with a distinct polarization direction. By applying electrical biasing or mechanical stressing, the polarization direction of these domains can be manipulated or switched. Understanding the behavior of ferroelectric domain switching under external stimuli is crucial for the development of ferroelectric-based technologies such as memories, actuators, and nanoelectronic devices.

In this presentation, we will discuss our recent in-situ transmission electron microscopy investigation of the effects of separate and combined mechanical and electrical loadings on ferroelectric domain structures. Our results demonstrate that mechanical confinement during electrical loading provides an additional degree of freedom for domain manipulation, which could significantly improve the performance of ferroelectric devices. We also found that a high-energy electron beam can precisely and reversibly control ferroelectric nano-domain morphology for memory storage devices by causing local accumulation of trapped charges that change the local electric field and, therefore, the local domain configuration.

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KL10 Molecular electronics: from fundamentals to materials

Elena Gorenskaia, Paul J. Low[1]*

[1]*School of Molecular Sciences, University of Western Australia*

**Email: paul.low@uwa.edu.au*

Molecular Electronics is a field of research and endeavor that explores the use of molecules to modulate the passage of electrical charge between two electrodes. Originally conceived in the 1950s, molecular electronics research has passed through several phases of interest, coinciding with developments in chemical design concepts in the 1970s and methods for contacting single-molecules by macroscopic electrodes and measuring the electrical properties of these single-molecule as well as 'large area' monolayer film based molecular junctions through the 1990s and 2000s, coupled with increasingly sophisticated theory and modelling.[1] Whilst initially envisioned as a route to miniaturization of electrical components (e.g. wires, switches, rectifiers and transistors), more recently interest in molecular electronics has expanded to wider applications, including green and bio-degradable electronics,[2] sensors [3] and energy materials.[4] This presentation will summarise advances in molecular designs for electronic components,[5] underpinned by advances in the development and verification of molecular circuit laws drawn from scattering models.[6] Beyond such scattering effects, the role of quantum interference effects on coherent charge transport will be demonstrated,[7, 8] and implications for such structure-property relationships in the design of molecular thermoelectric materials will be discussed.

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KL11 Resolving polydopamine structure: when theory guides experiment

Katya Pas,[1]* Sophie Crouch,[1] William Drury,[1] Ben Freeman[2]

[1] School of Chemistry, Monash University
[2] Centre for Water and Energy Systems, McKetta Department of Chemical Engineering, University of Texas at Austin
**Email: katya.pas@monash.edu*

Polydopamine (PDA) is a nature-inspired adhesive biopolymer that possesses a unique ability to adhere to any surface and form coatings that can withstand harsh environmental conditions.[1] PDA exhibits an array of attractive properties including electric conductivity, mechanical strength, antimicrobial activity, and antifouling, thus making it the sought-after polymer in industrial applications. As PDA is insoluble in all traditional aqueous and organic solvents, there is ambiguity surrounding its structure. It is not surprising that PDA is one of the most widely researched polymers, with thousands of papers published every year in attempt to bring more understanding towards its structure resolution.

Polydopamine is polymerized from dopamine dissolved in water under basic conditions. The solution turns black instantaneously, with solid aggregates precipitating out of the solution. Only very few initial steps of polymerization have been confirmed, including the cyclisation of dopamine and the formation of indole-5,6-qiuonone (IQ) and 5,6-dihydroxyl-indole (DHI). Over the years a myriad of structures has been proposed for the solid aggregates. In our group we designed quantum chemical calculations to understand the intermolecular interactions between monomeric units of dopamine – IQ and DHI – and potential ionic solvents.[2,3] 1-ethyl-3-methyl-imidazolium acetate ([C_2mim][Ace]) was predicted to be able to pull the monomeric units apart due to a strong interaction between the indole ring and the imidazolium cation. Subsequent dissolution experiments confirmed that [C_2mim][Ace] could indeed dissolve powered PDA, thus allowing us to perform ^{1}H NMR experiments and confirm the structure of PDA. In this talk I will present the details of how the structure was resolved and how this resolution served as the basis for parametrization of polarizable force fields to predict the dissolution and aggregation behavior of PDA and analogous polymers of the catecholamine family.

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KL12 Perovskites for electrochemical clean enegy and enviroment

Zongping Shao
[1] *WASM: Minerals, Energy & Chemical Engineering, Curtin University, Perth, WA 6402, Australia*
Corresponding author's email: zongping.shao@curtin.edu.au

Perovskites are a type of functional materials with the nominal ABX_3, where A can be rare earth elements, alkaline earth elements and even organic group, B site is usually transition metal elements, and X can be O^{2-}, S^{2-}, I^-, Br^- and F^-. In this presentation I will summarize our recent advances in the development of perovskite-type oxides for various clean energy and environment-related application, from solid oxide fuel cells, electrochemical and thermochemical water splitting for hydrogen production, advanced oxidation for waste water remediation, solar cells, and supercapacitors for energy storage (1-3), . The rational designs of perovskite-type functional materials for various applications, the advanced characterizations and device development will be mainly discussed, and future perspectives will also be proposed.

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KL13 Understanding battery materials during function and their thermal response

Neeraj Sharma[1]*

[1] *School of Chemistry, UNSW Sydney, Sydney NSW 2052, Australia*
Email: Neeraj.sharma@unsw.edu.au

Lithium-ion batteries are ubiquitous in society in applications ranging from portable electronics to electric vehicles and grid-scale electricity storage. They rely on electrochemical reactions at the electrodes which result in changes in the crystal structure of the active electrode materials via lithium-ion insertion/extraction. These changes directly impact the performance of such batteries and can be correlated to reversible energy storage density and lifetime. Synchrotron X-ray and neutron diffraction can be used to probe these changes and allow for atomic-scale monitoring of electrodes within devices during function. The first part of this presentation will showcase recent results from such experiments, investigating commercially-used electrode materials such as $LiNi_xMn_yCo_zO_2$ (NMC) and newly developed materials such as disordered rock salt oxides.

The insertion/extraction of lithium ions also changes the composition of the electrodes. From a structural chemistry point-of-view the lithium-ion inserted/extracted compositions are “new” compositions that can be explored, and their phase diagrams mapped. Our work has focused on the temperature dependent structural and phase evolution of the electrodes at various states of lithium-ion insertion/extraction. Similar work can be undertaken in sodium- and potassium-ion batteries and therefore phase space as a function of ion-type, ion insertion/extraction amount and temperature can be elucidated. Notably, in some cases new phases are found and this process of controlled alkali-ion insertion/extraction followed by thermal treatment has been coined as electrochemically activated solid state synthesis. The second part of this presentation will showcase studies of some conventional electrode materials and some more unusual electrodes that we have investigated, highlighting the thermal evolution and in some cases formation of new and unexpected phases.

Overall, this talk will highlight the rich structural chemistry that is present in alkali-ion batteries and how the understanding of such chemistry can be used to improve battery performance and even generate new materials.

KL14 Sean Smith (TBA)

KL15 Understanding the role of porosity, redox and acid sites in hydrodeoxygenation of biooils

Michael Stockenhuber[1]*

[1] *Chemical Engineering, The University of Newcastle, Australia.*
**Email: Michael.stockenhuber@newcastle.edu.au*

For modern energy applications with small or negative carbon footprint utilising unconventional renewable and sustainable sources new catalytic process technology has to be developed. In particular moving away from low oxygen content hydrocarbon feedstock as found in conventional, non renewable sources is challenging and new chemical processes have to be developed. Current energy production mainly relies on acid catalysis. Future feedstocks will need different catalytic processes to deliver energy carriers and bulk chemicals important for a modern society. In particular, bulk chemicals manufactured as a by product of fuel production will increase in scarcity because of lower fuel production. In this paper, we report on our efforts to convert hydrothermal liquefaction oils into high value chemicals such as BTEX as well as fuels. Heterogeneously catalysed reaction technology was developed where the balance of acid and redox sites, careful catalyst preparation and operational parameters such as temperature and pressure enabled us to control selectivity in the hydrodeoxygenation reaction. The pore distribution and morphology was also shown to play a very important role in determining selectivitv[1]. Careful catalyst preparation can significantly affect dispersion which in turn affects selectivity and activity[2]. The detailed chemical properties of catalysts[3], acidity[4] and promoters[5] all play an important role in reduction as well as cracking reactions[6] over heterogeneous catalysts. For example, we will report on a new generally applicable method to prepare transition metal zeolites which can improve metal dispersion and in turn control product selectivity and yields for a developed biocrude upgrade process[2]. In this lecture, we demonstrate how the development of a fundamental understanding of acidic, redox properties and pore morphology in microporous and mesoporous catalysts leads to the improvement of heterogeneous catalytic processes to sustainably produce aviation fuel and single ring aromatics.

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KL16 Engineered carbon nitride for energy and environmental catalysis

Hongqi Sun[1]*

[1]*School of Molecular Sciences, The University of Western Australia, Perth, WA6009, Australia*
**Email: hongqi.sun@uwa.edu.au*

The activity, selectivity and stability are determined by photocatalyst materials. Graphitic carbon nitride has been demonstrated to a promising catalyst for visible light photocatalysis. Compared to metal-based semiconductors, the polymeric semiconductor of carbon nitride has a low band gap energy, metal-free nature, easy preparation, and excellent catalytic activity. The small surface area and slow charge separation have restricted its photocatalytic applications. Tailoring its structure and composition, it is possible to make it efficient for a range of energy and environmental applications via photocatalytic redox reactions. In this talk, carbon nanospheres were prepared to attach on the graphitic carbon nitride, and the derived hybrids showed excellent efficiency in photocatalytic degradation of organic pollutants.[1] One-dimensional single walled carbon nanotubes (1D SWCNTs) were used to participate the thermal condensation of melamine, followed by thermal etching to prepared 1D SWCNT/2D C_3N_4. The novel photocatalyst demonstrated efficient activity for overall water splitting.[2] The 2D/2D van der waals heterojunction was achieved by a gas erosion processes on the exfoliated g-C_3N_4.[3,4] Furthermore, C_3N_4/graphene in-plane heterojunction was also designed, and the formation process was investigated in detail.[5] The studies show that metal-free carbon nitride-based hybrid materials can be designed for a variety of applications, such as photocatalytic degradation, selective oxidation, and water splitting, showing great potentials as excellent energy materials.

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KL17 Hydrogen storage and separation in porous materials for sustainable energy applications

Prof Valeska P Ting, [1,2]*

[1] Research School of Chemistry, The Australian National University, Canberra ACT 2601, AUSTRALIA
[2] College of Engineering, Computing and Cybernetics, The Australian National University, Canberra ACT 2601, AUSTRALIA
**Email: valeska.ting@anu.edu.au*

The impact of anthropogenic climate change has driven the development of hydrogen as an alternative low carbon energy vector. Hydrogen is globally abundant, is an extremely lightweight fuel with excellent energy density, and can be directly burned as a fuel or converted to electricity via a fuel cell with no harmful emissions. High surface area nanoporous materials such as porous carbon nanomaterials, zeolites and metal-organic framework materials are well suited for applications in hydrogen separation and storage. Their nanoscale and macroscopic structures can be tuned to allow exceptionally high densities of gas within their pores, which can lead to exciting possibilities for energy storage, both by physical adsorption of hydrogen and through emergence of unusual materials states via gas densification. It can, however, be extremely challenging to characterise and study interactions of H2 with nanoporous host materials due to hydrogen's low electron density, which makes it difficult to detect in the presence of heavier elements using X-ray techniques. Here we will present results from various studies, highlighting different approaches for extracting key information on the interactions between hydrogen and a range of porous materials. These include parametric studies and combinations of techniques including neutron scattering under static and dynamic conditions, gas sorption, molecular modelling and properties measurements under coupled extremes of low temperature and high pressures. Such studies can produce surprising and useful insights into the effect of nanoconfinement on the atomic arrangement, preference and properties of hydrogen under extreme environmental conditions, paving the way for developing new materials for sustainable energy applications.

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KL18Two-dimensional materials for next-generation electronics and optoelectronics technologies

Sumeet Walia [1]*

[1] *School of Engineering, RMIT University, Melbourne, Australia*

**Email: sumeet.walia@rmit.edu.au*

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

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

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

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

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KL19 Engineering of plasmoinc nanomaterials for surface-enhanced raman scattering-based *in vitro* cancer diagnosis

Yuling Wang [1*]

[1] *School of Natural Sciences, Faculty of Science and Engineering, Macquarie University, 2109, Australia*

**Email: yuling.wang@mq.edu.au*

Abstract: Cancer is a heterogeneous disease, which manifests as different molecular subtypes due to the complex nature of tumor initiation, progression and metastasis [1]. Non-invasive analysis of cancer biomarkers is in high demand and important for cancer diagnostics because it is the key to achieve the original and intact information from the cells. Thus, non-invasive and *in vitro* analysis of circulating biomarkers has the benefit of rapid, low-cost and little inconvenience to the patients. However, the achievement of in vitro cancer diagnosis is challenging due to the rare amount of cancer-relevant target biomolecules against an abundant background of non-biotargets. To overcome this technical hurdle in liquid biopsies, we have proposed and utilized surface-enhanced Raman scattering (SERS) spectroscopy as a new analytical tool for in vitro cancer diagnosis, owing to the ultra-sensitivity and multiplexing capability of SERS [2-3].

As plasmonic nanomaterials are the most common Raman signal amplifiers, advances in plasmonic nanomaterials play critical roles in facilitating SERS applications in cancer diagnosis. We thus have developed a few new strategies to engineer the functional plasmoinc nanomaterials for SERS-based *in vitro* cancer diagnostic application. In this contribution, I will present our recent results [4-8] in this evolving field—from the synthesis of cutting-edge plasmonic nanomaterials [4-5] to the design of biosensor platform [6-7] towards the comprehensive clinical evaluation of SERS strategies in cancer diagnosis.

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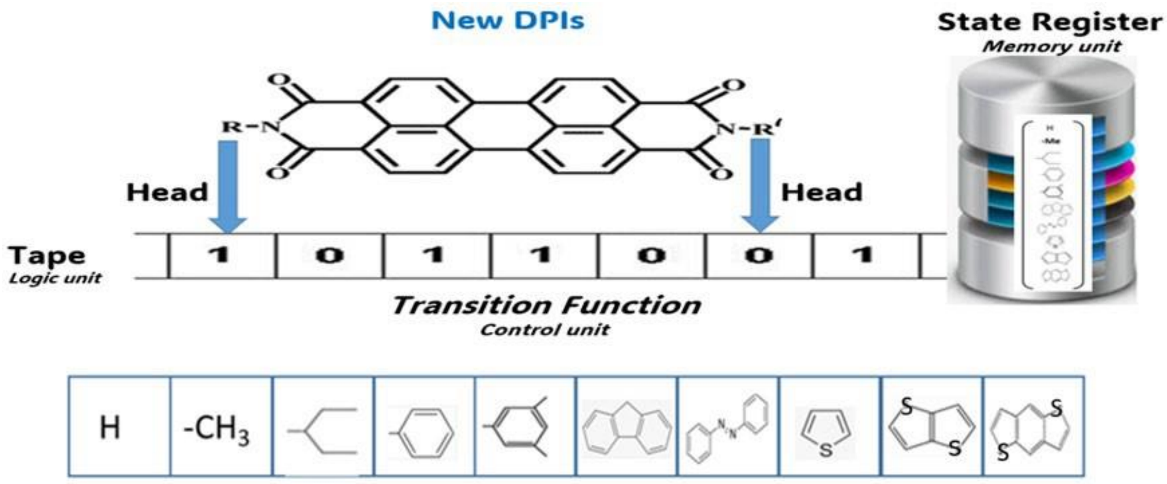
KL20_Intelligent design high performance PDI based dyes in solar cell applications

Feng Wang (王凤)[a,*] and Vladislav Vasilyev[b]

[a]*Department of Chemistry and Biotechnology,*
Swinburne University of Technology, Melbourne, Victoria 3122, Australia.
[b]*Australian National University*

**Email:* fwang@swin.edu.au

This study turns the design and screen of new compounds into a computer integer crunch of the control arrays using a scaffold based Turing machine model. If small organic fragments are stored in a fragment database (FDB) in which each fragment is labelled by an integer in an array, the position and frequency of the integer control how the fragment clicks on a scaffold (template compound). This method can robustly screen a large number of candidate fragments for solar cells and other applications such as drug design with minimal human assistance. As a proof of concept, we consider terminal imide substituents on the core perylene diimide (PDI) to develop PDI derivatives capable of absorbing UV-vis light for solar cell applications. Time dependent-density functional theory (TD-DFT) method was employed in the calculations. When the imide substituents are electron donors such as azobenzene (DPI-7), they produce a larger bathochromic shift (Δλmax) from the core DPI band position. The UV-vis absorption transitions of these DPI derivatives have more charge transfer (CT) character, as the highest occupied molecular orbitals (HOMO) are located on the fragments rather than the core DPI region. Our study presents a robust and efficient high-performance organic dye screen design strategy, and further research in DPI- based solar cell design will focus on promoting the HOMO to LUMO transitions of the optical spectra.



KL21 Design of micromotors for environmental applications

Shaobin Wang

[1] *School of Chemical Engineering, The University of Adelaide, Adelaide, SA 5005, Australia*
**Email: Shaobin.wang@adelaide.edu.au*

Artificial self-propelled micromotors with an asymmetrical structure can swim in a liquid solution under physical/chemical stimuli (e.g., light, ultrasound, magnetic field, temperature, and H_2O_2, etc.). As a green chemical, hydrogen peroxide can be decomposed by various metal-based materials (e.g., Pt, Ag, and MnO_2, etc.), and generate O_2 bubbles to drive micromotors. Owing to high catalytic activities and biocompatibility, MnO_2-based materials have shown advantages in the H_2O_2-fueled micromotors. Meanwhile, H_2O_2 decomposition to O_2 is competitive in producing hydroxyl radicals in Fenton reactions, which can be used for oxidation of environmental contaminants.

In recent years, we have carried out several investigations on synthesis of MnO_2-based micromotors by different techniques and also investigated their performances in simultaneously self-propelled motion and oxidative degradation of water contaminants. We found that MnO_2-based micromotors can be synthesized with varying properties and that they can catalyze different oxidants to induce various reactive species for organic decomposition.

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KL22 Corrosion behaviour of titanium alloys fabricated by additive manufacturing

Lai-Chang Zhang*
Centre for Advanced Materials and Manufacturing, School of Engineering, Edith Cowan University, 270 Joondalup Drive, Joondalup, Perth, WA 6027, Australia

** E-mail: l.zhang@ecu.edu.au*

ABSTRACT

Additive manufacturing technology can efficiently fabricate complex parts in near-net shape because it does not need to process molds and subsequent processing technology in component production. Additive manufacturing technology has become a research hotspot in recent years. Compared with traditionally prepared titanium alloys, 3D printed titanium alloys generally exhibit higher strength and plasticity. Since titanium alloys are often used in working environments with corrosive atmospheres, it is particularly important to study the corrosion behavior of 3D printed titanium alloys. However, there are very few studies on the corrosion behavior of 3D printed titanium alloys. This talk reports the corrosion behavior of various titanium alloys prepared by 3D printing technology (e.g., selective laser melting, electron beam melting). Studies have shown that the corrosion behavior of 3D printed titanium alloys is directly related to the 3D printing process and the microstructure of the fabricated alloy.

KL23 Bioinspired nanomaterials for drug delivery

Professor Chun-Xia Zhao[1,2]

1. Australian National Health and Medical Research Council (NHMRC) Leadership Fellow, Deputy Director of the Australian Research Council (ARC) Centre of Excellence; Professor at School of Chemical Engineering, University of Adelaide
2. Honorary Professor, Australian Institute for Bioengineering and Nanotechnology, University of Queensland.

Email: chunxia.zhao@adelaide.edu.au

Nanotechnology holds great promise for diagnosis and disease treatment. A wide variety of nanoparticles have been developed ranging from polymer particles to lipids, proteins and other synthetic compounds for drug delivery. Several different types of nanomedicines have been approved by the FDA, including liposome-based cancer nanomedicine, Doxil, protein-based cancer nanomedicine, Abraxane, and the very recent mRNA lipid nanoparticle COVID-19 vaccines. However, several key barriers need to be addressed: (1) challenges in large-scale production of nanomedicine with good reproducibility and well-controlled properties; (2) incomplete understanding of the interactions between nanoparticles and biological systems; (3) targeted delivery. To address these fundamental issues, my group has been focusing on the development of platform technologies for producing nanoparticle libraries with reproducible and systematically varied properties (lipid nanoparticles, polymer nanoparticles and nanocapsules) with tunable drug loading (up to 65%). We also developed different strategies for improving targeted delivery. Particularly, we developed a bioinspired nanotechnology integrating naturally derived cell membranes for enhanced the biointerfacing capabilities and nanoparticles for incorporation of various payloads for targeted delivery, which provides a revolutionising strategy for fabricating nanoscale artificial cells. We developed biomimicking chips (Tumor-on-a-Chip, Tumor-Vasculature-on-a-Chip) to fundamentally understand nanoparticle extravasation and their tumor accumulation. We also collaborate extensively with Australian companies for developing stable mRNA vaccines and personalised mRNA cancer vaccines.

ABSTRACTS FROM INVITED LECTURE (IL)

IL01	Dr. Sherif Abdulkader Tawfik Abbas	Deakin University
IL02	Dr. Lei Bao	RMIT University
IL03	Nigel Brand	Potable Spectral Service
IL04	Dr. James Bullock	The University of Melbourne
IL05	Prof Neil Cameron	Monash University
IL06	Dr. Samuel Cheeseman	The University of Melbourne
IL07	Dr. Dechao Chen	Griffith University
IL08	Dr. Peng Chen	The University of Queensland
IL09	Dr. Fangfang Chen	Deakin University
IL10	Prof. Zhenxiang Cheng	University of Wollongong
IL11	Prof Dewei Chu	University of New South Wales
IL12	Prof. Hui Tong Chua	The University of Western Australia
IL13	Kristoffer Collopy	Adoxima Pty Ltd
IL14	A/Prof. Torben Daeneke	RMIT University
IL15	A/Prof. Raffaella Demichelis	Curtin University
IL16	A/Prof. Wei Deng	University of Technology Sydney
IL17	Dr. Patrick Doheny	The University of Sydney
IL18	Dr. Wesley Dose	University of New South Wales
IL19	Dr. Xiaoguang Duan	The University of Adelaide
IL20	Dr. Alison Edwards	ANSTO
IL21	Dr. Aaron Elbourne	RMIT University
IL22	A/Prof. Terry Frankcombe	University of New South Wales
IL23	Dr. Changkui Fu	The University of Queensland
IL24	Dr. Qiang Fu	University of Technology Sydney
IL25	A/Prof. Alf Garcia-Bennett	Macquarie University
IL26	Dr. Lucy Gloag	University of Technology Sydney
IL27	A/Prof. Alexey Glushenkov	Australian National University
IL28	A/Prof. Matthew Griffith	University of South Australia

IL29	Prof.	Lisbeth	Grondahl	The University of Queensland
IL30	Dr.	Qinfen	Gu	ANSTO
IL31	Dr.	Zhaojun	Han	University of New South Wales
IL32	Dr.	Junnan	Hao	The University of Adelaide
IL33	A/Prof.	Daniel	Heath	The University of Melbourne
IL34	A/Prof.	Min	Hong	University of Southern Queensland
IL35	Dr.	Long	Hu	University of New South Wales
IL36	Dr.	Xiaodan	Huang	The University of Queensland
IL37	Dr.	Xia	Huang	The University of Queensland
IL38	A/Prof.	Franca	Jones	Curtin University
IL39	A/Prof	Rakeshi	Joshi	University of New South Wales
IL40	Dr.	Mega	Kar	Deakin University
IL41	Dr.	Eleanor	Kearns	The University of Sydney
IL42	Dr	Muxina	Konarova	The University of Queensland
IL43	Prof.	Yeng Ming	Lam	Nanyang Technological University
IL44	A/Prof.	Guoliang	Yang	Deakin University
IL45	Dr.	Haiyan	Li	RMIT University
IL46	Prof.	Wenxian	Li	University of New South Wales
IL47	Dr.	Mengyao	Li	University of New South Wales
IL48	Dr.	Gemeng	Liang	The University of Adelaide
IL49	Dr.	Rijia	Lin	The University of Queensland
IL50	Prof.	Christopher	Ling	The University of Sydney
IL51	A/Prof.	Dan	Liu	Deakin University
IL52	A/Prof.	Yazi	Liu	Nanjing Normal University
IL53	Dr.	Teng	Lu	Australian National University
IL54	A/Prof.	Jennifer	MacLeod	Queensland University of Technology
IL55	Dr.	Jianfeng	Mao	The University of Adelaide
IL56	Dr.	Jacob	Martin	Curtin University
IL57	Prof.	Anthony	Masters	The University of Sydney
IL58	Dr.	Karolina	Matuszek	Monash University

IL59 Dr. Yuan Mei CSIRO
IL60 Dr. Izaac Mitchell Curtin University
IL61 A/Prof. Stephen Mogach The University of Western Australia
IL62 Dr. Fatemah Mokhtari Deakin University
IL63 Dr. Hieu Nguyen Australian National University
IL64 Prof. Alister Page University of Newcastle
IL65 A/Prof. Weikong Pang University of Wollongong
IL66 Prof Adam Perriman Australian National University
IL67 Dr. Charlotte Petersen The University of Melbourne
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IL70 Dr. Neil Robinson The University of Western Australia
IL71 Dr. Stephen Sanderson The University of Queensland
IL72 Dr. Ryan Shaw Thermofisher
IL73 Dr. Cameron Shearer The University of Adelaide
IL74 Dr. Peter Sherrell RMIT University
IL75 Dr. Xiaolei Shi Queensland University of Technology
IL76 Dr. Chien-Chung Shih National Yunlin University of Science and Technology
IL77 Prof. Prashant Sonar Queensland University of Technology
IL78 Prof. Pingan Song University of Southern Queensland
IL79 Dr. Peter Spackman Curtin University
IL80 Prof. Michelle Spencer RMIT University
IL81 A/Prof. Dawei Su University of Technology Sydney
IL82 Xueqian Sun Australian National University
IL83 Dr. Bing Sun University of Technology Sydney
IL84 Prof. Yasuhiro Tachibana RMIT University
IL85 Prof. Youhong Tang Flinders University
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IL87 Prof. Richard Tilley University of New South Wales

IL88 Dr. Nevena TodorovaRMIT University

IL89 Prof. Antonio Tricoli The University of Sydney

IL90 Dr. Bryan Tuten Queensland University of Technology

IL91 Dr. Tao Wan University of New South Wales

IL92 A/Prof. Yun Wang Griffith University

IL93 Dr. Yichao Wang Western Sydney University

IL94 Dr. Liang Wang Griffith University

IL95 Dr. Li Wei The University of Sydney

IL96 A/Prof. Asaph Widmer-Cooper The University of Sydney

IL97 Dr. Sandra Wiedbrauk Queensland University of Technology

IL98 Prof. Chaoyu Xiang Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences

IL99 Prof. Haolan Xu University of South Australia

IL100 Dr. Xiaomin Xu Curtin University

IL101 Dr. Pei Lay Yap The University of Adelaide

IL102 A/Prof. Jiabao Yi University of Newcastle

IL103 A/Prof. Huacheng ZhangRMIT University

IL104 Prof. Rongkun Zheng The University of Sydney

IL105 Dr. Yijun Zhong Curtin University

IL01 The power of physics-informed machine learning in solving nanoscale challenges

Sherif Abdulkader Tawfik Abbas[1]*, Tri Nguyen[1], Truyen Tran[1], Sunil Gupta[1] and Svetha Venkatesh[1]

[1] Applied Artificial Intelligence Institute (A2I2), Deakin University, Australia
**Email: s.abbas@deakin.edu.au*

Machine learning (ML) has undoubtedly contributed to a revolution in material science. The exponential increase in publications over the last decade demonstrates the diversity of problems which ML could solve, or potentially solve. Underpinning the success of ML are major advances in material featurisation (the description of a material to ML models).[1] However, physics-informed ML models have very recently started topping the charts.[2–4] These are deep ML models that benefit from the injecting physical insights into the model's fabric. Here I demonstrate how insights from density functional theory (DFT) were able to improve the accuracy of ML models. I will introduce our direct integration of interatomic potentials (DIIP), a novel approach to include physics into deep ML models. We implement our DIIP physics-informed ML method within a number of deep graph neural network (GNN) models.[5] Training DIIP is performed at our institute's GPU cluster. We generate a dataset of DFT properties for > 10,000 materials using VASP. We benchmark our new model using the MaterialsProject, JARVIS and QM9 benchmark datasets. DIIP achieves a mean absolute error (MAE) of 0.033 eV and 0.037 eV in predicting the formation energy and total energy, respectively, and outperforms ALIGNN[6] in predicting the bandgap (3% improvement). I will demonstrate the application of DIIP for predicting the properties of new 2D materials. The inclusion of more relevant physics into GNNs improves the accuracy of ML for predicting material properties, and enables the bespoke discovery of new classes of nanomaterials.

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IL02 Surface nanodroplet confined engineering of gold nanostructures

Lei Bao1*

[1]*School of Engineering, STEM College, RMIT University, Melbourne, Vic 3000, Australia*

**Email: lei.bao@rmit.edu.au*

Surface nanodroplets are referred to as small droplets with attoliter to femtoliter in volume and immobilised on substrates in contact with an immiscible liquid phase. The unique microenvironment of surface nanodroplets renders advanced features for miniaturising processes and reactions with high efficiency[1,2]. The liquid-liquid interface between nanodroplets and the surrounding phase allows for extended droplet lifetime as well as for reagents imparting from one phase to the other. Within droplets, reactions are compartmentalised and accelerated due to the high surface area-to-volume ratio of nanodroplets[3].

In this work, we show the in situ formation and assembly of gold-thiolate nanostructures in surface nanodroplets. Each droplet served as a nanocompartment to confine the nucleation and growth of the gold nanomaterials. The as-formed gold-functionalised droplets can facilitate a catalytic reaction, leading to a fast fluorescent quench of Nile Red accumulated in droplets.

Moreover, we show that after exposure to air, the shrinking of these gold-thiolate decorated droplets led to assembled gold-thiolate nanostructures on the surface. The composition of droplets and the substrate wettability are both key elements to alter these assemblies. The obtained gold-thiolate complex with active gold atoms can serve as scaffolds to enable the selective growth of gold spikes on the top, which have been regarded as favourable structures for surface-enhanced Raman scattering (SERS) substrates[4]. Our results herein highlight the potential of surface nanodroplets as novel miniaturisation platforms for nanomaterial synthesis, nanostructure fabrication, and catalytic reaction in nanoscale.

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IL03 Materials Chemistry – A Micro-XRF Perspective

Dr Nigel Brand, [1]*,

[1] *Portable Spectral Services*
[2] *Adjunct Fellow, University of Western Australia*
**Email: nwbrand@portaspecs.com*

In the dynamic landscape of contemporary challenges and escalating demand for material discovery and characterization, the need for a rapid, nondestructive technique elucidating detailed material chemistry and mineralogy has become paramount. Micro-XRF technology addresses this imperative by facilitating rapid, high-resolution scans with minimal sample preparation, offering an environmentally friendly solution devoid of chemicals. Applicable in both academic and industrial contexts, as well as field settings, this technology provides rapid, real-time information.

Its unique capacity to analyse large samples, up to 7 kg, "as is" without preparation, unveils material structures and impurities in direct relevance to the original composition. This talk by Portable Spectral Services will showcase examples illustrating the diverse applications of Micro-XRF technology, spanning biological samples to critical minerals. By connecting these examples to your current material research we aim is to inspire the integration of this technology into your future research and development workflows.

IL04 van der Waals Materials for Infrared (IR) Photodetection

James Bullock, 1*

[1] *Department of Electrical and Electronic Engineering, University of Melbourne, Victoria 3010, Australia*

**Email: james.bullock@unimelb.edu.au*

Layered van der Waals materials have shown promise for use in short-wave to long-wave IR photodetectors. One of the key advantages offered by layered materials is their out-of-plane van der Waals bonding which allows the use of thin layers without suffering from detrimental effects such as surface dangling bonds. This advantage is particularly important in IR detectors where thin absorbers can reduce volume dependent noise, a strategy which is often not permitted in traditional semiconductors due to surface recombination. In this talk, we present some of our recent results on the development of IR photodetectors based on low dimensional materials [1-5]. Black phosphorus (bP) is among the highest performing van der Waals materials, already being demonstrated in devices yielding room temperature detectives of ~10^{10} Jones in the mid-wave IR region. The success of bP has prompted its incorporation into a broad range of advanced optical structures including in Fabry-Pérot cavities [5], on photonic circuit waveguides [2], and also as dual-color bias-selectable detectors [1]. In addition to bP, we also introduce some of our recent results on newer van der Waals materials for IR photodetection, such as $ZrGeTe_4$ [4].

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IL05 Cardiac tissue engineering scaffolds by 3D printing with multilayer polymer composites

Muthu V. Vellayappan[1], Francisco Duarte[1], Cyrille Sollogoub[2], Alain Guinault[2], Justin Dirrenberger[2], Jessica Frith[1], Andrey Molotnikov[1,3,4], Helena C. Parkington[5], Neil R. Cameron[1,6]*

[1]Department of Materials Science and Engineering, Monash University, 14 Alliance Lane, Clayton, VIC 3800, Australia
[2]PIMM, Arts et Metiers Institute of Technology, CNRS, Cnam, HESAM University, 151 boulevard de l'Hopital, 75013 Paris (France)
[3]Monash Centre for Additive Manufacturing (MCAM), 11 Normanby Road, Nottinghill, VIC, 3168, Australia
[4]RMIT Centre for Additive Manufacturing, School of Engineering, RMIT University, Melbourne, Australia
[5]Department of Physiology and the Biomedicine Discovery Institute, Monash University, Victoria, Clayton, Australia
[6]School of Engineering, University of Warwick, Coventry CV4 7AL, UK
**Email: neil.cameron@monash.edu*

The past two decades have witnessed increasing evidence that the mechanical properties of biological tissues is pivotal for cellular behaviour and tissue functionality. This knowledge, along with previously known contact guidance, has immensely advanced the field of cardiac tissue engineering. However, the synergistic effect of contact guidance and material stiffness on cellular behaviour in a co-culture setting is still unclear because we lack fabrication techniques that can produce tissue-engineering scaffolds with simultaneous periodic stiffnesses and topographies. Here, we present a simple fabrication method for the creation of advanced all-polymer composite scaffolds via multi-layer co-extrusion and fused deposition modelling 3D printing. Extensive characterisation of the composite materials by a suite of chemical and imaging methods reveals that the multi-layered architecture is preserved after printing, and results in architectured composite scaffolds. These scaffolds are used to investigate simultaneously mechanotaxis and contact guidance of cardiomyocytes and fibroblasts in vitro. Cell-scale topography and alternating polymer stiffness improved cell alignment and preferential migration. Functional analyses revealed spontaneously active, synchronous, and rhythmic cardiomyocytes contraction. Thus, we demonstrate a simple and inexpensive strategy to produce multilayered polymer composite scaffolds for cardiac tissue engineering.

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IL06
Samuel Cheeseman, The University of Melbourne
TBA

IL07 Ligand mediated surface engineering of environmentally friendly quantum dots

Dechao Chen, [1]*, Qin Li[1]

[1] Queensland Micro- and Nanotechnology Centre, Griffith University, Brisbane, QLD 4111, Australia
*Email: Dechao.chen@griffith.edu.au

Ligand mediated surface engineering is a powerful approach to manifest the physical and chemical properties of quantum dots. [1-3] We present a general top-down and bottom-up method to attract and assemble high-quality carbon dots and zinc-based quantum dots through a colloidal synthesis strategy. The colloidal synthesis improved the quality of quantum dots in its size control and uniformity. The colloidal quantum dots showed an improved emission profile and interesting photophysical properties. The results revealed the surface ligand function and interactions. Benefitting from the outstanding optical and colloidal stability, the colloidal quantum dots demonstrated excellent potential in photo energy conversion applications.

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IL08 Phase stabilization strategies for efficient perovskite solar cells

Peng Chen*, Lianzhou Wang*

Australian Institute for Bioengineering and Nanotechnology and School of Chemical Engineering, The University of Queensland, Brisbane, Australia
**Email: p.chen1@uq.edu.au, l.wang@uq.edu.au*

The recent decade has witnessed the rapid increase in the power conversion efficiency of metal halide perovskite solar cells (PSCs) from 3.8% to certified 25.7%. Despite their success in achieving intriguing photovoltaic performance, the inferior phase stability of PSCs against external stimuli (e.g. moisture and UV light) remains a critical hurdle for their further large-scale applications. Herein, we introduced innovative strategies, including interfacial engineering,1-2 surface ligand decoration,3 and material composition,4 to stabilize the photoactive phase and simultaneously passivate surface defects of perovskites for optoelectronic applications. By rational design on interfacial and surface engineering, the fabricated PSCs delivered a champion power conversion efficiency of 23.89%, which can be retained 90% after aging in a humid atmosphere (relative humidity level 60%) for 1,000 hours. 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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IL09 A comparison of constant charge and constant potential models in investigating ionic liquid electrolyte-electrode interface

Fangfang Chen, * Jhonatan Soto Puelles

[1] Deakin University (Burwood Campus), 221 Burwood HWY, Burwood, 3125
**Email: fangfang.chen@deakin.edu.au*

Understanding electrolyte-electrode interfacial nano structures and chemistries is particularly important in the field of batteries and supercapacitors. In batteries, the electrolyte naturally forms a layered structure near the charged electrode surface due to a charge screening effect. Next to the negatively charged anode, the electrolyte will decompose through redox reactions, forming an electronic insulate and ion conductive layer, named the Solid Electrolyte Interphase (SEI). This layer will ultimately prevent further decomposition of the electrolyte. Therefore, it is crucial to battery stability, safety and life. Understanding the SEI formation is a major challenge in battery research due to its complexity.

Since the innermost electrolyte layer next to the anode is the first place where the electrolyte decomposition occurs, the information of this layer will provide us with the first clue to the SEI formation. Our previous research has shown that the composition of this layer is affected by many factors, including electrolyte compositions, electrode chemistry and applied current density [1-3], indicating that good SEI could potentially be designed through pre-conditioning processes targeting different electrolyte compositions. Molecular simulation plays a significant role in this study. Two types of electrode models are commonly adopted for this study, the constant charge model and the constant potential model. In the first model, the atomic charge is uniformly distributed on the surface atoms of electrode to give a constant charge density. The advantage of this model is the low computational cost. In the second model, a constant potential is given to the electrodes while allowing the surface charge oscillation. This model is closer to the real situation, but with a dramatically increased simulation cost. In this talk, I will present a comparison between two models in investigating the interface between a hybrid ionic liquid/organic solvent electrolyte and the gold electrodes.

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IL10 Tunning of electron configurations in transition metal oxides for higher OER

Zhenxiang Cheng
Institute for Superconducting and Electronic Materials, Innovation Campus, University of Wollongong, North Wollongong, NSW 2500, Australia
E-mail: cheng@uow.edu.au

Electrocatalytic water splitting holds great promise for the future energy conversion devices, but the kinetics of the sluggish oxygen evolution reaction (OER, $4OH^- = O_2 + H_2O + 4e^-$) is the rate-determining step and deserves to be studied extensively. The oxygen evolution reaction process not only requires four sequential proton-coupled electron transfers, but also includes a transition in the spin states. Such a spin state transition needs to be promoted by additional energy to occur, enough voltage together with spin orbital coupling.

Considering the scarcity and high cost of commercial OER catalysts, such as Pt and magnetic RuO_2/IrO_2, a great deal of effort has been expended on possible alternatives. Transition metal-based perovskite is one of the most excellent candidates, owing to its abundance, relatively good stability, and benign electrocatalytic active. In 2011, a volcano-shaped curve of OER efficiency against the number of eg electrons of surface transition metal cations has been proposed by Yang Shao-Horn et al. Following this rule, the fastest OER is observed on $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe0.2O_{3-\delta}$ (BSCF), of which the magnetic ions are in the intermediate spin state, that is, the number of eg electrons is around 1.2. Since then, this principle has become an effective guideline to improve the efficiency of perovskite oxide OER catalysts.

Since then the eg electron rule has fully demonstrated its power in OER process. Interestingly, the electron configuration of transition metals also decides the magnetic property of the compounds and finally the electron transfer in the catalytic process. In this talk, using a few examples of transition metal based OER catalysts I will demonstrate how the electron configuration of transition metal decides catalytic behavior, the spin state transition during OER process and the possible approaches to facilitate the transition.

IL11 Bio-inspired nanoionic materials for energy &information related device applications

Dewei Chu
School of Materials Science and Engineering, UNSW Sydney
*Email: d.chu@unsw.edu.au

Inspired by nature, we have developed new nanoionic materials and devices which can mimic the functions of human brain and skin with low power consumption through engineering the ion migration in nanoionic devices. For example, a new design of artificial perceptual system integrating ZnO-based synaptic devices with Pt/carbon nanofibers-based strain sensors for stimuli detection and information processing is presented. The device can emulate various essential functions, such as short-term/long-term plasticity, paired-pulse facilitation, excitatory post-synaptic current, and synaptic plasticity depending on the number, frequency, amplitude, and width of the applied pulses.

Inspired by Harvesting energy from ubiquitous moisture is attracting growing interest for wearable electronics. However, it is still challenging to fabricate high-performing moisture-electric generators (MEGs) with high and stable electric output. Herein, we report a facile strategy to modify the oxygen-based groups of graphene oxide using acid treatment, which boosts the electric output based on the device structure of graphene oxide/polyvinyl alcohol (GO/PVA) MEGs. Furthermore, the electrode configuration has been optimized to enhance the power output. This work may open a new era of advance for a new energy conversion technology able to directly power wearable electronic devices.

IL12 Production of few-layer graphene and boron nitride nano onions via lamp ablation

Jijiang He [1,2,+], Hongyu Zhang [1,2,+], Weike Zhang [3,4], Jeffrey M Gordon [5], Hui Tong Chua [1,*]

[1] Department of Chemical Engineering, The University of Western Australia, Perth, WA 6009
[2] Ablano Pty. Ltd., 5 Lindsay Street, Perth, WA 6000, Australia
[3] School of Materials Science and Engineering, Taiyuan University of Technology, Taiyuan 030024, China
[4] Energy Research Institute at NTU (ERI@N), Nanyang Technological University, 1 Clean Tech Loop #06-04, Singapore, 637141
[5] Department of Solar Energy and Environmental Physics, Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede Boqer Campus 8499000, Israel
[+] Equal first author
**Email: huitong.chua@uwa.edu.au*

Few-layer graphene, and separately, boron nitride nano onions have been synthesised by a novel lamp ablation method which is a one-step, high-yield process that is catalyst-free, devoid of toxic reagents, with short reaction times, and potentially scalable [1,2]. The precursor for the few-layer graphene is graphite flake, while that of boron nitride nano onions is hexagonal boron nitride powder. Product nanostructures are characterised by high-resolution transmission electron microscopy (HRTEM), energy-dispersive X-ray spectroscopy (EDS), electron energy loss spectroscopy (EELS) and scanning electron microscopy (SEM). The few-layer graphene products, in dry powder form, are further characterised by atomic force microscopy (AFM) and Raman spectroscopy and determined to be 7-8 layer thick. For the boron nitride nano onions, an array of characterisation procedures revealed nanoparticle (a) shapes and sizes, morphing from polyhedral for diameters of order 10^1 nm to quasi-spherical at diameters of order 10^2 nm, and (b) composition, with a 1:1 B:N ratio while also confirming the absence of contaminants. A formation mechanism is proposed whereby boron nitride nano onions evolve from the initial thermal exfoliation of the bulk precursor powder into nano-platelets. They fold and close into hollow nanocages that are more stable thermodynamically. We also report on our commercialisation trajectory to translate promising research findings in the laboratory to the market. For both the few-layer graphene and boron nitride nano onion products, they are presently on a pre-commercial pilot plant phase.

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IL13 DNC technology: Nanotechnology master process for the scalable production of advanced materials

Kristoffer Collopy | Director | Adoxima | 0422 593 059

**Email:* kris@adoxima.com

Adoxima Pty Ltd has achieved a breakthrough in the material manufacturing industry with our cutting-edge DNC™ Technology. The DNC™ Technology platform enables us to mass-produce a vast spectrum of specialty oxide materials, varying in complexity, while maintaining a high degree of consistency in their properties.

Adoxima is in the process of scaling-up the synthesis of boehmites and pseudoboehmite – very-high-purity hydrated aluminas (aluminium oxihydroxide). These are commonly used as precursors in the production of various advanced ceramics, catalysts, and other high-performance materials. New advancements in various fields have showcased the versatility of these aluminas, extending their usage to a diverse range of applications, including catalysts, automotive coatings, adjuvants, composites, lithium-ion battery separators (LIBS), and printed circuit boards (PCB).

Adoxima is also testing its process to design products for new market applications such as hydrogenation catalyst, rubber industries, cement industries and the like. An exciting development is that we have recently been able to craft a cutting-edge Aluminium oxyhydroxide vaccine adjuvant. This innovative product showcases substantial progress in essential characteristics crucial for the development of more potent vaccines. These include improved surface to volume ratio, purity, colloidal suspension and high antigen absorption.

IL14 Liquid Metals – A unique class of catalysts for CO_2 reduction and NH_3 synthesis

<u>Torben Daeneke</u>[1]* Ken Chiang[1], Karma Zuraiqi[1], Dan Yang[1], Mariam Ameen[1]

[1] RMIT University, School of Engineering, 124 LaTrobe Street Melbourne
**Email: Torben.daeneke@rmit.edu.au*

Liquid metals are an emerging class of compounds that are liquid close to room temperature yet exhibit metallic conductivity[1]. Liquid metals are truly multifunctional and over the past years, liquid metals have not only been used for the design of flexible and reconfigurable electronics but also emerged as a platform for the synthesis of 2D materials at their surfaces [2,3], nano-structures in their bulk [4] and as a unique class of catalysts that are extraordinarily resilient towards deactivation and feature surprising catalytic activity [5]. In comparison to other liquids such as covalent solvents and ionic liquids, comparatively little is known about the chemistry that occurs in molten metals. This talk covers the emerging picture of liquid metal chemistry and will also introduce some of our recent results in the area of CO_2 reduction to graphene and NH_3 synthesis [6].

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IL15 Modelling the dynamics of molecules with conformational freedom in water: the example of aspartic acid

Alicia Schuitemaker,[1,2] Katarzyna B. Koziara,[2] Paolo Raiteri,[2] Julian D. Gale[2] and Raffaella Demichelis,[2,]*

[1] ARC Centre of Excellence in Exciton Science,
School of Chemistry and The University of Sydney Nano Institute, University of Sydney, NSW, Australia
[2] School of Molecular and Life Sciences, Curtin University, Perth, WA, Australia
**Email: raffaella.demichelis@curtin.edu.au*

An accurate atomic-scale analysis of the dynamics of aspartic acid species and of their association with calcium ions in water at pH values relevant to biomineralization will be presented.

A new classical model was developed[1] and applied to calculate ion pairing profiles, obtaining ion pairing free energy values that are in agreement with experiments. The model was then used to probe the stability of aqueous homochiral and heterochiral clusters, which are claimed to form and act as growth modifiers during the formation of calcium carbonate.[2,3]

Results show that modelling molecules with conformational freedom in the context of biomineralization comes with additional levels of complexity, due to different conformations being more or less stable depending on whether the molecule is free or bound. In fact, if the rotational free energy barrier is high, an appropriate bias needs to be added to accelerate the torsional dynamics. This aspect is rarely considered in molecular simulations of mineral-organic interfaces and can significantly affect both the quality and accuracy of the results.

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IL16 Light-triggered liposome system for targeted gene editing

Yagiz Alp Aksoy[1], Biyao Yang[2], Ewa M Goldys[2] and Wei Deng[3]*

[1]Diabetes and Metabolism Division, Garvan Institute of Medical Research, Sydney, NSW, Australia;
[2]the Graduate School of Biomedical Engineering, University of New South Wales, Australia
[3]the School of Biomedical Engineering, University of Technology Sydney, NSW, Australia
Email: Wei.Deng@uts.edu.au

The current in vivo CRISPR therapeutics largely relies on biological deliver agent (“viral vector”) which passively deliver and release the CRISPR without tumor-targeting capability. This fact causes the tissue-specific off-target issue, a major challenge affecting the clinical translation of in vivo CRISPR therapeutics. Despite huge interest in liposome/lipid delivery systems (non-viral vector) for CRISPR-related applications, there is a research gap in development of spatiotemporal controlled CRISPR release. We developed a light-sensitive liposome delivery system that offers a high degree of spatial and temporal control of gene editing with CRISPR/Cas9 system. In this work we achieved light-triggered liposomes by incorporating a photosensitive molecule, verteporfin (VP) inside the lipid bilayer. Under light illumination at 690 nm wavelength, VP reacts with available oxygen molecules and generates singlet oxygen which oxidises the unsaturated lipid components and leads to destabilisation of the liposomal structure and CRISPR release. We demonstrated its high transfection efficiency, by assessing the targeted knockout of GFP gene in human HEK293 cells (52.8% knockout). We further validated our results at a single-cell resolution using an in vivo GFP reporter system in zebrafish (77% knockout). In vivo gene editing benefits from organ-specific targeting to prevent undesirable off-target gene editing events. Spatial and temporal control of gene editing using the liposomal delivery platform we developed (patented) will open new options for exciting science and wider translation of targeted CRISPR-based gene therapy.

IL17 Investigations of a 2d co(ii) system on a highly frustrated triangular lattice

Patrick W. Doheny,[1] Gavin B. G. Stenning,[2] Fabio Orlandi,[2] Pascual Manuel,[2] Sam T. Carr[3] and Paul J. Saines[1]

[1] *School of Chemistry and Forensic Science, Ingram Building, University of Kent, Canterbury, CT2 7NH, United Kingdom*
[2] *ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom*
[3] *School of Physics and Astronomy, Ingram Building, University of Kent, Canterbury, CT2 7NH, United Kingdom*
**Email: P.Saines@kent.ac.uk*

Magnetic frustration, where magnetic spins cannot adopt a single, low energy ground state, is responsible for a number of novel and exotic magnetic properties.[1] Such frustrated materials, whose magnetic properties are thought to enable new methods of spin control, are of great interest to emerging applications such as spintronics, quantum computing and quantum data storage.[2] One method of designing such quantum materials is to engineer them on geometrically frustrated lattices where the arrangement of the magnetic components leads to competing, magnetically frustrated interactions. Despite this, the fundamental properties and behaviour of such magnetically frustrated materials are often poorly understood, which impedes steps towards the concerted design of quantum materials for real-world applications. This presentation will detail the investigation of a 2D Co(II) material which crystallises in a layered, triangular lattice geometry.[3] Magnetic susceptibility and heat capacity measurements demonstrate that this S = 3/2 system experiences a high degree of magnetic frustration with a calculated frustration index of f = 73. Neutron powder diffraction data, collected at 87 mK, allowed the magnetic structure of the material to be solved which revealed a collinear ferromagnetic arrangement of Co(II) spins. The origin of the observed magnetic frustration, which was seemingly contradicted by the ferromagnetic structure solution, is likely to arise from dimensional crossover due to the influence of interactions in the 3rd dimension on the highly frustrated antiferromagnetic layers.

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IL18 Understanding degradation in lithium-ion batteries

Wesley Dose

School of Chemistry, University of New South Wales, Sydney, Australia
Email: wesley.dose@unsw.edu.au

Battery technologies are critical for Earth's low carbon future. Lithium-ion batteries, already widely used in portable electronics, are the dominant technology for the rapidly growing electric vehicle and grid scale energy storage markets. This growth requires the aggressive optimization of the cost, energy density, power density, cycle life, safety, and sustainability. Layered oxide positive electrodes with high nickel (and low cobalt) content have emerged as a promising class of materials for the next generation of batteries, however, the poor cycle life hampers the adoption in commercial cells.[1,2] Understanding the material degradation mechanisms is a crucial first step towards developing practical solutions. This talk will describe how a combination of tailored electrochemical protocols, microscopy, spectrometry, and spectroscopy can be used to explore electrode, electrolyte, and interface degradation. First, we discuss degradation initiated by cycling to high voltage and the important role played by the electrolyte.[3,4] Next, a mechanism for synergistic degradation at high and low voltage will be outlined.[5] Finally, the detrimental impact of material degradation on the capacity retention and cell impedance will be discussed along with a perspective on promising avenues to mitigate the degradation.

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IL19 Single atom catalyst for photo-Fenton-like reactions

Xiaoguang Duan [1]*

[1] *School of Chemical Engineering, The University of Adelaide, SA 5005, Australia*
**Email: xiaoguang.duan@adelaide.edu.au*

In this work, we developed a series of structure-well-defined carbon-based single-atom catalysts (SACs) to replace conventional metal/semiconductor counterparts and drive several key processes in photocatalytic 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 heterogeneous and photocatalysis. We found that SACs can effectively activate various peroxides to generate reactive oxygen species (ROS) under light irradiation 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 heterogeneous/photo-catalytic behaviors 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 solar driven oxidation technology to secure water safety in the post-COVID era.

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IL20 Single-Crystal neutron diffraction KOALA2 leads the way!

Alison J Edwards, Ross O Piltz

Australian Centre for Neutron Scattering, ANSTO, Lucas Heights, NSW 2234
**Email: Alison.Edwards@ANSTO.gov.au*

Historically, neutron single-crystal diffraction was a technique available for materials characterization in the most limited of circumstances, access to a suitable neutron beam, availability of a suitable instrument with detector and the existence of a single-crystal of sufficient size. A resurgence of the Laue method in structure determination occurred in the late 20th century was facilitated by increased computational capacity and driven by the recognition of the potential that the use of white-beam methodologies. The first suite of neutron beam instruments at the OPAL reactor included KOALA[1] – a single-crystal Laue diffractometer which became a dominant instrument in neutron single-crystal chemical crystallography and materials characterization – our success has been underpinned by the development of LAUEG[2] which allows users to extract routine data from images and can be used by experts to unravel more challenging problems. As the electronic components of the instrument aged, it became clear that a new control system was required, and ultimately we have been fortunate to be funded to design and build a completely new instrument – KOALA2 which incorporates significant improvements over the original. Much of the design work was completed through online collaboration during COVID lockdowns and the build was achieved away from the instrument enclosure minimising the loss of beam access. KOALA2 is now in user operation less than a year from the last experiment conducted on KOALA and data collected in the first month of operation is expected to be published in Tier One chemistry journals in early 2024. We anticipate that KOALA2 will continue to lead the way in single-crystal neutron diffraction over the next decade or more. The instrument is near full subscription until the 2024 long shut-down – watch for the 2024 proposal round for longer term work, but please be aware that some discretionary time is available for urgent cutting-edge work!

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IL21 Behaviour of citrate-capped gold nanoparticles at biomembranes – atomic insight at supported lipid bilayer and liposome interfaces

Aaron Elbourne [1,*] *Rashad Kariuki,*[1] *Rowan Penman,*[1] *Saffron J. Bryant,*[1] *Rebecca Orrell-Trigg,*[1] *Nastaran Meftahi,*[2] *Russell J. Crawford,*[1] *Christopher F. McConville,*[1,3] *Gary Bryant,*[1] *Kislon Voïtchovsky,*[4] *Charlotte E. Conn,*[1] *Andrew J. Christofferson,*[1,2]*

[1] School of Science, STEM College, RMIT University, Melbourne VIC 3001, Australia.
[2] ARC Centre of Excellence in Exciton Science, School of Science, RMIT University, Melbourne, VIC 3001, Australia.
[3] Deakin University, Geelong, Australia.
[4] University of Durham, Physics Department, Durham DH1 3LE, UK.

**Email: aaron.elbourne@rmit.edu.au*

Introduction: Nanomaterials - materials with nanoscale dimensions - are widely investigated, especially in many biological settings. This is due to their potential use as advanced nano-medicines and diagnostic technologies, antimicrobials, as cellular probes, and in cellular-imaging, among other applications. The commonality between all applications is that they utilise the nanosized features of the material, specifically their departure from traditional bulk-like properties. In general, nanoparticle-based biotechnologies must interact with, and often cross, a cellular membrane to be useful; however, the dynamics of these interaction is still poorly characterised.

Aim: Combine advanced experimental and computation studies to study the interaction of ultra-small gold nanoparticles (AuNP) at a synthetic bio-membrane to see 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 were used to study the fundamental behaviour of the AuNPs at the bio-membrane-liquid interface. The systems of interest are models consisting of supported lipid bilayers (SLBs) (see Figure 1.) and free-floating liposomes. These act as archetypal bio-membranes. Liquid-phase, ripple-phase, and gel-phase biomembranes were used to systematically asses interactions.

Results: We investigated the behaviour - dynamics, adsorption, translocation, and physical interactions – of a variety of AuNPs at the biomembrane interface. The techniques listed above are beginning to provide localised, 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 behaviours: 1) initial adsorption, 2) nanoparticle incorporation and/or translocation, 3) particle-induced phase change, and 4) translocations of the particles. These interactions are of broad scientific and medical interest because nanomaterials have recently become a viable method for manipulating matter at the cellular level, particularly for therapeutic and diagnostic applications.

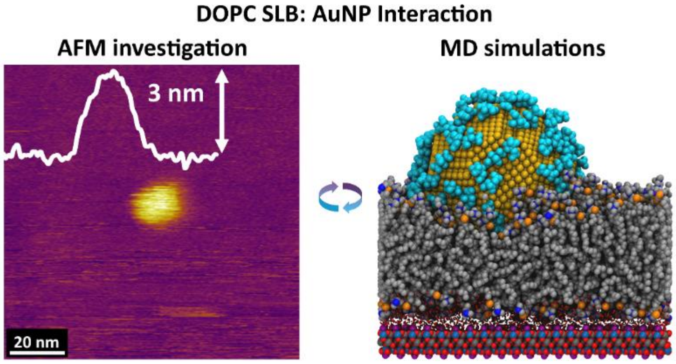

Figure 1. AFM (left) and MD simulations (right) of AuNP-SLB interaction.

IL22 Simulating X-ray photoelectron spectra

Terry J. Frankcombe

University of New South Wales, Canberra
**Email: t.frankcombe@adfa.edu.au*

X-ray Photoelectron Spectroscopy, or XPS, is a powerful experimental technique for probing elemental and ionic compositions of solids. Under X-ray bombardment, the kinetic energies of photoelectrons emitted from core states reveal information about the oxidation state of the parent ions as well as the surrounding material environment. Each element gives XPS signals at particular energies, that vary predictably with oxidation state. While DFT methods have developed to the point where XPS spectra can be predicted with high accuracy for molecular species, this is more difficult for crystals and surfaces. In this work we calculate core state energies using a number of different DFT packages, and use their energies relative to well-defined, self-consistent reference states to predict XPS spectral features. For example, the lattice oxygen of metal oxides typically gives a strong XPS signal at 530 eV from 1s electrons. The 1s orbital energies of slabs of material can be used to demonstrate that an XPS signal at 531 eV does not come from "oxygen deficient regions" (a.k.a. lattice oxygen vacancies) [1] as was suggested by Fan and Goodenough more than 45 years ago [2]. This incorrect assignment has been used widely over the past few decades. In this talk I will give an overview of this work and some other recent results.

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IL23 Antifouling and antibacterial polymers and surfaces

Xin Xu, Yuhao Zhang, Yutong Gong, Peng Hui, Andrew Whittaker, Changkui Fu[1]*

[1]Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St. Lucia, Queensland 4072, Australia

Email: changkui.fu@uq.edu.au

Biofouling caused by nonspecific adsorption of biomolecules and organisms such as proteins, cells, and bacteria to material surfaces is a significant challenge for numerous important applications. Many strategies have been used to combat biofouling. Polymers have been playing significant roles in modulating material-bio interactions and impart desired antifouling and antibacterial properties. Developing new functional polymers that possess superior antifouling and antibacterial properties and understanding the structure-property relationship in such polymers is therefore greatly demanded.

In this presentation, I will introduce a new class of antifouling and antibacterial sulfur-containing polymers, and highlight some important effects such as polymer identity and microstructure on the antifouling and antibacterial performance of the polymers and polymer-modified surfaces.

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IL24 Nanoengineered membrane materials of energy and environmental applications

Qiang Fu[1]*

[1] *The Centre for Technology in Water and Wastewater (CTWW), School of Civil and Environmental Engineering, University of Technology Sydney (UTS)*

**Email: qiang.fu@uts.edu.au*

The emission of CO2 to the atmosphere from the use of fossil fuels has been linked to global climate change. As estimated by the International Energy Agent (IEA), fossil fuels fulfilled 81% of the world energy demand in 2013.[1] Among various CCS approaches, post-combustion CCS is the most urgent one since it can be directly retrofit to existing fossil fuel-fired power generators.[2] Membrane technology has been considered as an economic and energy-saving alternative capture strategy to solvent scrubbing for the mitigation of CO2 from post-combustion exhaust gas (10-14% CO2 with mostly N2).[3] Permeance and selectivity are the two major criteria to evaluate the performance of any CO2 separation membrane system. However, common dense membranes display insufficient capability for CO2 capture due to their overall low flux (permeance) of CO2.

Thin film composite (TFC) membranes can facilitate high CO2 permeation and hence are of potential significance for large scale application which requires the treatment of high-volume flue gases in comparison with conventional membranes. The great challenge in assembling TFC membranes is to reduce the overall gas transport resistance without compromising membrane selectivity.[4] In order to minimise the resistance, we designed and constructed a series of TFC membranes consisting of a porous MOF gutter layer and a nano-scale top selective layer.[5,6] Such TFC membranes present extremely high CO2 permeance with a good CO2/N2 selectivity. This performance is well above the boundary of the well-known target area for post-combustion CO2 capture applications.

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IL25 Protein corona mediated biological properties of mesoporous silica particles

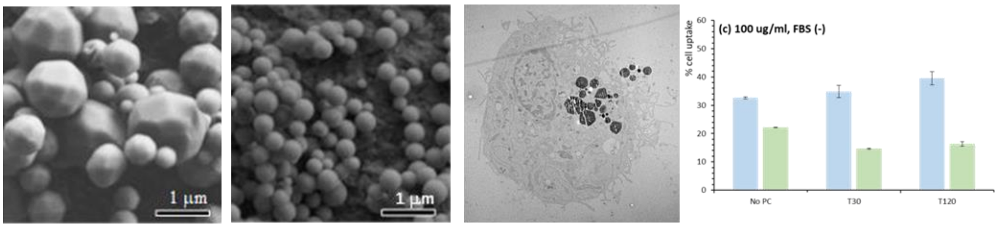
Alfonso E. Garcia-Bennett, [1,2]*, Michael Lau[1]

[1] School of Natural Sciences, Macquarie University, Sydney, 2109 NSW, Australia.
[2] ARC Training Centre for Facilitated Advancement of Australia's Bioactives, Macquarie University, Sydney, 2109 NSW
**Email: alf.garcia@mq.edu.au*

Mesoporous silica particles (MSPs) excel in oral, transdermal, ocular and for intraperitoneal drug formulation.[1] When colloidal particles are dispersed in physiological media, they exhibit a high degree of protein opsonization resulting in the formation of an enzymatic or protein corona (PC) surrounding the particle. The new bio-molecular corona that ensues, largely affects the function of the MSPs.[2]

The PC interferes with drug release properties and therapeutic efficiency, cellular uptake, and the particle's immunological properties. We perform characterization of the soft and hard corona focusing on particle morphology, cell uptake and cytotoxicity effects to understand the PC of MSPs,[3] and its potential role in mediating immunological properties.[4-6]

Our results conducted with spherical and facetted particles of the MSP known as AMS-6 suggest that the particle morphology can determine the size and type of PC, which consequently has a strong influence on the cell uptake, viability and biological properties of this type of mesoporous silica. We show evidence for the role of the PC through a range of material and biological characterization techniques including biological assays and pharmacokinetic *in vivo* data.



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IL26 Electron microscopy for electrocatalytic materials

Lucy Gloag[1]*

[1] *School of Mathematical and Physical Sciences, University of Technology Sydney, Sydney, NSW 2007*
**Email: gloaglucy@gmail.com*

Electrocatalysts are used for >80% of catalysis in chemical manufacturing processes and are one of the key components in water storage and conversion technologies that are set to play a major role in Australia's National Hydrogen Strategy by 2030.[1] The field of materials chemistry has been dominated by the development of highly efficient electrocatalysts. We are now at a point where materials are being synthesized with atomic level precision, resulting in the most active, stable, and selective electrocatalysts. [2,3] This is the end result of materials synthesis, characterization and electrocatalytic advancements occurring simultaneously over decades.

The development of electron microscopy techniques has been central to the advancement of electrocatalyst materials synthesis and design. In this presentation, the interdependence of characterization methods with synthetic and electrocatalytic progress will be discussed. I will outline how the resolution, speed and accessibility of electron microscopy techniques has dictated nanomaterials research over the years and led research to the state-of-the-art atomically precise electrocatalyst materials.

As we move forward to create the next generation of electrocatalysts with even more advanced structures and properties, we need to consider integration of theoretical and synthetic protocols, precision in synthesis and characterization methods and advancements in-situ analysis.

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IL27 Assessment of dual-ion batteries with antimony-based and phosphorus-based anodes

Alexey M. Glushenkov,[1,2,*], Thrinathreddy Ramireddy[1,2]

[1] Research School of Chemistry, The Australian National University, Canberra, ACT 2601, Australia
[2] Battery Storage and Grid Integration Program, The Australian National University, Canberra, ACT 2601, Australia
**Email: alexey.glushenkov@anu.edu.au*

Dual-ion batteries represent an interesting detour from the conventional concept of “rocking chair” lithium-ion batteries. These batteries utilize similar organic electrolytes; however, the cathode operation relies on the intercalation of anions at high potentials. This allows the creation of batteries with higher cell voltage and a modified fast charge / high power profile. The studies globally are directed at various modifications of these batteries with the aim to understand these systems better.

Usually the concept of a dual-ion battery relies on graphitic negative electrode materials. These materials have attractive electrochemical performances but relatively limited theoretically available capacity (372 mAh/g). In principle, a different class of negative electrode materials that include Si, Bi, P, Sn, Sb, Al (these elements have an ability to alloy electrochemically with lithium) exists as an alternative to graphite and offers considerably larger capacities. Previously, our team has developed phosphorus- and antimony-based electrodes for lithium-ion batteries [1, 2] that can also be used in a dual-ion battery format.

This presentation will demonstrate the operation and performance of dual-ion battery full cells with phosphorus- and antimony-based anodes [3, 4]. Initially, the performance of individual electrodes (including graphite cathodes) is assessed in optimal electrolytes. The full cell dual-ion batteries are then designed with two different maximum cell voltages. The observed electrochemical behaviour is discussed and compared with that of a more conventional graphite-graphite full-cell dual-ion battery.

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IL28 Semiconducting polymer nanoparticles: enabling a new frontier in bioelectronic neural interfacing

Matthew J. Griffith,[1,2,]* Jessie A. Posar,[2] Natalie P. Holmes,[2] R. Crovador,[2] Connor P. Sherwood,[3] Paul C. Dastoor,[3] Alan M. Brichta,[3] and Rebecca Lim[3]

[1] Future Industries Institute, University of South Australia, SA, 5095, Australia
[2] School of AMME, University of Sydney, Camperdown, NSW, 2006, Australia
[3] School of Biomedical Sciences, University of Newcastle, NSW, 2308, Australia
**Email: matthew.griffith@unisa.edu.au*

Implantable neurostimulation devices play a key role in treating injuries and diseases, however, their progression out of the laboratory remains limited by a low biocompatibility that reduces *in vivo* device lifetimes, a mechanical rigidity that is poorly matched with soft tissue causing inflammation and ineffective electrical contact, and a requirement for costly external power supplies to deliver current.[1] These issues result in indiscriminate tissue activation, with a consequent lack of the required spatial selectivity.

In this work, we report our group's recent efforts to simultaneously address these issues by combining soft carbon-based organic semiconductors and nanoscale science to build new bioelectrodes that allow optical neurostimulation without external power. Our approach creates bioelectronic interfaces from conducting polymers that can be formed into customized nanoparticles with established solution-based chemistry methodologies. This approach enables the stimulating electrodes to be combined with targeted pharmaceutical factors in the fabrication procedure, which subsequently optimize connections to the neural network when released *in-vivo*.[2] We will discuss how we tuned the optoelectronic properties of the polymer nanoparticles to cover standard red, green, and blue spectral regions, allowing spectrally selective platforms for neurostimulation. These materials are then turned into electroactive inks, and subsequently fabricated into pixelated arrays using inkjet printing that demonstrate both anatomical and functional biocompatibility via immunolabelling with neuronal marker MAP2 and visualisation with epifluorescence microscopy. We demonstrate the controlled release of drugs from the organic semiconducting nanoparticles via electrical stimulation, aiding in precise spatial delivery of pharmaceutical factors. Finally, we employ whole-cell patch clamp electrophysiology recordings to demonstrate an exciting result; purely optical neurostimultation of dorsal root ganglion nerve cells. We demonstrate that the organic semiconductors can trigger changes in the nerve cell membrane potentials via a capacitive coupling mechanism, the efficacy of which can be improved by judicious selection of the device architecture.[3]

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IL29 Delivery of therapeutic agents using biopolymers

Lisbeth Grøndahl [1*]

[1]*School of Chemistry & Molecular Biosciences, The University of Queensland, Brisbane, Australia*
Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Australia
**Email: l.grondahl@uq.edu.au*

The use of delivery systems to deliver therapeutic agents is a strategy used to enhance drug stability, reduce side effects, and target specific sites. The applications that we have explored are vast and cover cancer therapy, tissue regeneration, and vaccines. Depending on the application, different administration routes are required which put restrictions on the type of delivery system that can be used both in terms of size and surface properties. The work presented will illustrate design parameters for delivery of a range of active agents, e.g. small organic molecules, proteins, oligonucleotides, polysaccharides. Biopolymer-based particles are the focus of the work encompassing polysaccharide, peptide and polyester based systems. Specific systems include bone-seeking chitosan nanoparticles used in cancer therapy; alginate submicron-sized particles used for tissue regeneration; layer-by-layer coated nanoparticles used for oral vaccine; poly(lactide-co-glycolide) nanoparticles in cancer therapy. The control of size and surface properties will be highlighted as will challenges and pitfalls in characterisation of the delivery systems; the effect of the release media; and the method of evaluating release of therapeutic agents.

IL30 Utilizing synchrotron technology for researching energy and environmental materials to shape our future

Qinfen Gu, [1]*, Anita D'Angelo[1], TAN, Liam[1], Helen Brand[1]

[1] *Australian Synchrotron, ANSTO*
**Email: qinfeng@ansto.gov.au*

In recent decades, there has been a growing interest in porous materials, notably metal-organic frameworks (MOFs) and zeolites, owing to their remarkable characteristics, including an exceptionally high surface area and customizable pore chemistry [1, 2]. MOFs and zeolites, for the most part, exhibit substantial pore volume and surface area, thus offering relatively high adsorption capacities for molecules and ions. However, these materials may still exhibit shortcomings in terms of their ability to effectively separate and adsorb substances. Consequently, there is a significant demand for the development of advanced methodologies for producing porous materials.

Synchrotron X-rays provide an intense beam that enables in-situ investigations of advanced materials for energy and environmental applications. Synchrotron facilities offer a variety of techniques through different beamlines, delivering structural and chemical insights across diverse time and length scales. As an illustration, in-situ powder X-ray diffraction (PXRD) uses the high intensity and resolution of synchrotron radiation for fast studies of the mechanism of several tailor-made advanced materials. Meanwhile, X-ray absorption spectroscopy (XAS) exploits the adaptable energy properties of synchrotron radiation to furnish information about interatomic distances, bonding valences, and oxidation states of the materials. This presentation will delve into a selection of case studies involving advanced materials designed for efficient separation and storage, carried out at the Australian synchrotron, showcasing the potency of these methodologies.

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IL31 Electrochemically synthesized H_2O_2 for environmental applications

Zhaojun Han [1,2,3,*]

[1] School of Chemical Engineering, University of New South Wales, Kensington, NSW 2052, Australia
[2] CSIRO Manufacturing, 36 Bradfield Road, Lindfield, NSW 2070, Australia
[3] School of Mechanical, Medical and Process Engineering, Queensland University of Technology, Brisbane, QLD 4000, Australia
**Email: zhaojun.han@unsw.edu.au; zhaojun.han@csiro.au; zhaojun.han@qut.edu.au*

Hydrogen peroxide (H_2O_2) is one of the most important and versatile industrial chemicals with widespread applications in environmental remediation, paper bleaching, and chemical synthesis. Industrial scale H_2O_2 is currently produced through the multistep anthraquinone oxidation process, which involves substantial energy consumption and waste generation. The transport, storage, and handling of bulk H_2O_2 also impose additional cost and safety issues. Recently, electrochemical synthesis became an attractive alternative to the energy-intensive anthraquinone oxidation process for on-site H_2O_2 generation. We demonstrate that metal-free carbon-based catalysts are promising in electrochemically synthesizing H_2O_2 at high efficiency: (i) oxygen-containing functional groups on the edges of vertical graphene are the active sites in catalytic reactions [1,2]; (ii) high activity and high selectivity can be achieved simultaneously in a flow cell with engineered three-phase interface [3]; (iii) N-doped carbon catalyst can result in a high concentration of >10,000 ppm; and (iv) in-situ generated H_2O_2 is further used to electrochemically synthesize a strong oxidant peracetic acid (PAA). Our results pave the way for decentralized, controllable and environmentally-friendly production of H_2O_2 that could be suitable for a variety of applications.

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IL32 New electrolytes and electrodes for aqueous Zn batteries

Junnan Hao [1]*, Shi-zhang Qiao [1]

[1] *School of Chemical Engineering and Advanced Materials, The University of Adelaide, Adelaide, 5005.*
**Email: Junnan.hao@adelaide.edu.au*

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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IL33 Improving biomaterials through the design of polymeric materials that enable control over the type and nano-scale presentation of cell-adhesive ligands

Fatemeh Karimi[1], Shirin Nour[2,3], Andrea J. O'Connor[2], Greg Qiao[3], Daniel Heath[2]*

[1] School of Biomedical Engineering, University of New South Wales, Kinsington NWS 2033
[2] Department of Biomedical Engineering, Graeme Clark Institute, University of Melbourne, Parkville VIC 3010
[3] Department of Chemical Engineering, Polymer Science Group, University of Melbourne, Parkville VIC 3010

**Email:* *daniel.heath@unimelb.edu.au*

Biomaterials are commonly functionalised with cell-adhesive ligands that regulate the cell-material interaction through engagement of cell surface receptors.[1] Traditionally, integrin receptors have received significant attention; however, other important cell receptors exist that have not been fully explored from a biomaterials perspective.[2] Additionally, most biomaterial interfaces are functionalised with the cell-adhesive ligands in a random manner; however, nanoscale pattering of the ligands at the biointerface can further regulate cell-material interactions by facilitating the formation of signaling complexes.[3] In this presentation, we will discuss our recent work on the development of polymeric biomaterial coatings that allow us to investigate the role of multiple cell adhesion molecules in regulating cell-material interactions through control of the type and nanoscale distribution of cell-adhesive ligands presented at the biointerface. Specifically, we will show that control of these parameters can improve cell adhesion rate, adhesion strength, proliferation, differentiation, and mechanotransduction.[4,5]

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IL34 Reinforcing phonon scatterings to enhance *zT*

Min Hong[1]*

[1] *Centre for Future Materials & School of Engineering, University of Southern Queensland, Australia*
**Email: min.hong@usq.edu.au*

The coupling relationships of thermoelectric properties make it challenging to enhance *zT*. Favourable, lattice thermal conductivity (κ_l) is independently governed by phonon transport.[1-2] A net increase in *zT* can be achieved by reducing κ_l. In our recent research outcomes, new mechanisms have been developed to reinforce phonon scattering. First, we introduced the concept of tuning phonon dispersion to enhance phonon-phonon scatterings in GeTe alloys.[3-4] By modifying the phonon dispersion, we were able to improve the scattering of phonons, leading to a reduction in κ_l. Additionally, in polycrystalline thermoelectric materials, to enhance the mid-frequency phonon scattering, we introduced high-density dislocations in the Bi_2Te_3 material through the mechanical plastic deformation and stacking faults in $AgSbTe_2$ by adjusting the synthesis method. Furthermore, we developed high-density planar vacancies and superlattice precipitates in GeTe alloys, leading to a significant reduction in κ_l. To gain a deeper understanding of the underlying connection between structural/lattice imperfections and low κ_l, we employed electron microscopy characterizations and first principle calculations.[5] By significantly reducing κ_l using these novel strategies, we have successfully enhanced *zT* in various materials. These rationally established approaches provide alternative routes to tailor the thermoelectric performance of various materials.

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IL35 Halide perovskite quantum dot electronics

Long Hu*, Tom Wu, Dewei Chu

[1] *School of Materials Science and Engineering, UNSW, Sydney*
**Email: long.hu@unsw.edu.au*

Halide perovskite quantum dots are one of promising materials for electronic device applications due to their excellent properties such as size and composition dependent bandgap tunability[1], ideal unity photoluminescence quantum yield[2], high defect tolerance[3] as well as low-temperature and solution processing[4].

Driven by these characteristics, this presentation will deliver high performing quantum dot electronics including solar cells and gas sensors through the strategies of materials synthesis, interfacial engineering, and surface modification.

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IL36 Origin and prevention of dendrites in aluminium metal anode containing electrochemical cells

Xiaodan Huang*, Dmitrii A. Rakov, Chengzhong Yu

Australian Institute for Bioengineering and Nanotechnology, The University of Queensland,
Brisbane, QLD 4072, Australia
**Email: x.huang@uq.edu.au*

The origin of dendritic short-circuiting in multivalent ion batteries with metallic anodes based on abundant elements, e.g., magnesium, calcium, aluminium and zinc, is relatively elusive compared to these understandings for alkali metals. Specifically, for aluminium-ion batteries (AIBs) this phenomenon questions the role of solid-electrolyte interphase (SEI) and its changes during the cycling. Here, we showed how applied electrical current controls the structure and ion dynamics at the electrified interface near aluminium anode to disclose conditions of SEI formation leading to irreversible cycling in AIBs. We found that unstable aluminium metal anode cycling occurs on the surface with a large portion of electrochemically inactive SEI components, e.g., oxide-rich, or solvent-derived-organic-rich interphases. In such conditions, the metal deposition is likely to happen locally at "electrochemically active sites" leading to the formation of metallic dendrites. These understandings propose new protocols for dendrite-free cycling of AIBs and highlight the importance between interfacial nanostructuring and interphase formation in multivalent-ion batteries.

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IL37 Materials for lithium-ion batteries

Dr. Xia Huang[1], Prof. Lianzhou Wang[1,2]*

[1] *Australian Institute for Bioengineering & Nanotechnology*
[2] *School of Chemical Engineering, The University of Queensland*
**Email: l.wang@uq.edu.au*

Transport electrification has been identified as an essential step towards energy transition from fossil fuels to renewable energy sources to reduce petroleum reliance and alleviate the associated environmental impacts.[1] Advances in lithium-ion battery (LIB) technology regarding energy density improvement and cost reduction are urgently needed to enable a deeper penetration of electric vehicles. The cathode materials of LIB not only set the energy density celling, but also dominate the cost of the current battery technology. Our research activities focus on the development of cathode materials that are composed of cheap elements (Mn-rich) and have high energy density (high specific capacity and/or high voltage).[2-5] Our efforts are to develop new and known materials leap forward in performance, while to gain a deep understanding of the structure-property-performance relationships through a wide range of materials and electrochemical characterizations.

Along with the bourgeoning LIB markets, opportunities and challenges emerge in the supply chains of battery. In addition to the pursuit of material frontiers, we also work closely with industries, such as making the low profit mining raw materials to high value-added electrode materials for LIBs & improving the electrode performance.

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IL38 Impact of stereochemistry on the formation of solids contributing to crystal arthritis

Franca Jones[1]*, Odin Botrill[1], Mauro Mocerino[1]

[1]Curtin University, Bentley, WA, Australia
**Email: F.Jones@curtin.edu.au*

Crystal arthritis is a medical term for conditions where crystals form within the joints of a **patient. These solids then cause significant swelling and pain for the patient.[1] Although** this condition is very widespread globally, especially in older patients, there are limited treatments and there is limited research into the impacts of organic additives on the formation and the resulting crystals. [2, 3] For crystal arthritis the most prominent crystal forms are monosodium urate (gout) and calcium pyrophosphate (pseudogout). The work presented here investigates L- and D-Proline as well as these molecules functionalized onto a calixarene 'scaffold' as possible crystal growth modifiers. This investigation should give insight into the role of stereochemistry and the impact of tethering these molecules to larger scaffolds.

It was found that the L- and D-Proline had unique interactions with the crystal formed in the medium as shown by XRD, IR, Raman, and SEM despite the small difference between the molecules. It appears that when present during the formation of monosodium urate, L-Proline results in sharper peaks (more ordered solids) in the XRD. Conversely, during calcium pyrophosphate formation L-Proline resulted in a broadening of peaks (more disordered solids) in the XRD. This confirmed the importance of stereochemistry on the crystallization process. The presence of L- and D- Proline calixarene compounds had different impacts during crystallisation compared to the pure amino acid at similar concentrations and again stereochemical specific effects were seen.

This research demonstrates that there is still much to learn about crystallisation as changing the stereochemistry of a chemical added into the medium can result in very different impacts on the crystal formed.

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IL39 Graphene oxide membranes for purification and separation

Rakesh Joshi*,

School of Materials Science and Engineering, University of New South Wales, Sydney, Australia
**Email:* r.joshi@unsw.edu.au

We report graphene oxide (GO) based membranes with proper control of structure and morphology for water purification, selective gas separation and moisture adsorption. We have investigated the water transport of cation-intercalated graphene oxide membranes. The cations act as water-attracting impurities on the channel walls. Via controlled water transport experiments, we show that the slip length of the nanochannels decays exponentially with the hydrated diameter of the intercalated cations. In collaborative projects with industries, we have successfully employed our GO membrane to remove natural organic matter and other species from water while maintaining high water flux. In addition, we introduce a straightforward electrochemical method utilizing the angstrom-confinement of laminar reduced graphene oxide (rGO) nanochannels to obtain a centimetre-scale network of atomically thin (< 4.3 Å) 2D-transition metal oxides (2D-TMO).

IL40 Advanced, non-aqueous electrolytes for rechargeable metal batteries

Mega Kar, [1]*, Douglas R MacFarlane[2], Dale Duncan[1], Binayak Roy[2], Maria Forsyth[1]

[1] Deakin University, Burwood Highway, Victoria, 3125, Australia
[2] Monash University, Wellington Road, Clayton, Victoria, 3800, Australia
**Email: m.kar@deakin.edu.au*

There is a critical need to design inexpensive, non-flammable and stable materials for the next generation of rechargeable batteries to overcome the variability of renewable energy in Australia. Metal batteries have come a long way since the 1920's since the progression in non-aqueous electrolytes have been employed to overcome safety concerns with moisture and air-sensitive metals, i.e. Li.

Recently, advanced electrolytes based on liquid salts have garnered enormous interest in the field of electrochemistry for energy storage technologies. Herein the design of a series of weakly-coordinating borate based electrolytes1-3, with low-volatility and high oxidative stability, is reported. Such materials make them immensely attractive for high-voltage cathodes. Moreover, their electrochemical compatibility with a number of various metals including lithium (Li), sodium (Na) and magnesium (Mg) is demonstrated, making them highly appealing for a number of emerging rechargeable metal battery technologies such as high-energy density batteries based on Li as well as affordable, safer alternatives such as sodium and magnesium.

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IL41 3D printing of metal-organic framework composite materials for electrochemical and direct air capture applications

E. R. Kearns[1,2*], Marcello B. Solomon[1,2], Qingbo Xia[2], Nicholas Proschogo[2], Rohan Gillespie[3], D. M. D'Alessandro[1,2]

[1] School of Chemical and Biomolecular Engineering, The University of Sydney
[2] School of Chemistry, The University of Sydney
[3]Southern Green Gas
**Email: ekea7127@uni.sydney.edu.au*

Additive manufacturing is a powerful technique allowing access to novel and unique geometries of materials. When additive manufacturing is combined with advances in novel materials, such as Metal-Organic Frameworks (MOFs), highly specialised devices can be created.[1] MOFs are a class of highly porous crystalline materials; their modular and tuneable structure allows MOFs to be specifically tuned to certain applications.

In this presentation, two different 3D-printed devices containing MOFs as the active component are reported. The first is a 3D-printed lattice, fabricated by Direct Ink Writing, which shows significant promise for application in the Direct Air Capture of carbon dioxide. By incorporating carbon additives into the system, an in-built resistive heating capability is accessed. The second device manufactured is an electrode for sensing and electrocatalysis applications. The unique structures of the incorporated MOFs make these electrodes extremely sensitive and selective for the analyte of choice.

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IL42 Enabling hydrogen storage and transport: unleashing cost-effective potential through liquid organic hydrogen Carriers

Muxina Konarova

School of Chemical Engineering, The University of Queensland
Brisbane Qld 4072 Australia
Email: m.konarova@uq.edu.au

Liquid Organic Hydrogen Carriers (LOHCs) stand out as one of the most economical and safe alternatives for hydrogen transportation. This technology, relevant at large scale, relies on a hydrogen carrier's cyclic hydrogenation (LOHC→LOHC+) and dehydrogenation (LOHC+→ LOHC). However, nowadays, the hydrogenation of the LOHC still requires a source of H2, with high purity, i.e., >99%, and pressure, e.g., P ≥ 30 bar. Thus, simply transporting H2 via LOHC will not turn the economic scales of H2 widespread usage. The main reasons for using pure H2 for hydrogenation are related to metal-based catalyst stability, as is the high H2 pressure [1]. Indeed, typical impurities in raw H2-rich streams from biomass include CO and H2S (known poisons for most metal catalysts), H2O (promotes metal sintering), CO2 (can be transformed via H2 over metal-based catalysts into CO, H2O, and CH4, decreasing H2 recovery and causing catalyst deactivation), CH4, and other inert gases, like N2. Therefore, the development of stable catalysts in the presence of raw H_2 impurities and under milder conditions would open the door for direct use of LOHC hydrogenation. Hydrogenation of organic molecules require metal particles to be present in the catalyst, these are now exclusively dedicated to activating H2 molecules which mainly focused on noble metals such as Pt on alumina, Pd on sodalite [2]. These noble metals were encapsulated in small pore zeolites to prevent the deactivation of the metallic phase by poisoning, sintering, and coke deposition. Nowadays, no catalyst exists to use LOHC hydrogenation for effective raw H2 purification. While hydrogen splitting over Pt/zeolites can be a viable solution, these noble metals are expensive and very sensitive to impurities. In addition, the most Pt/zeolite -based catalysts for LOHC reaction suffers from coking and thus require frequent regeneration by burning the coke which will make significant amount of CO2 and metal sintering/loss of surface area. In this talk, types of catalysts suitable for liquid organic hydrogen carriers will be presented, with a focus on hydrogenation of N-ethylcarbazole using catalysts.

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IL43 Materials Strategies for Hybrid Perovskite Devices

Yeng Ming Lam[1,2], Hongwei Hu[1,3], Tze Chian Sum[4], Haixia Rao[1], Senyun Ye[4]

[1]School of Materials Science and Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798.
[2]Facility for Analysis, Characterisation, Testing and Simulation (FACTS), Nanyang Technological University, 50 Nanyang Avenue, North Spine, Block N4.1-B4-10, Singapore 639798
[3]Institute of Intelligent Flexible Mechatronics, Jiangsu University, 212013, Zhenjiang, China
[4]Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371
E-mail: ymlam@ntu.edu.sg

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 how facile is the methodology. In this presentation, two examples will be shown on how the understanding of the materials can lead to simple solution with good outcome. 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 Pb^{2+} or Sn^{2+}, 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. Hybrid perovskites also have shown to have great potential to be used as emitters with tunable emission, high colour purity and good ease of fabrication. A lot of studies have so far been focused on three-dimensional (3D) perovskites, such as $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ for green and infrared emission. The organic molecules used in these systems can be varied and it can give rise to different optical behaviour. I will also share some work that we have done with active cations which of energy levels that can be made use of to encourage the harvesting of triplets and this opens up a very interesting optoelectronic behaviour.[2]

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IL44 Functional nanomaterials for water and energy harvesting

Guoliang Yang[1], Weiwei Lei[1*]

[1]Institute for Frontier Materials, Deakin University, Waurn Ponds Campus, Locked Bag 20000, Victoria 3220, Australia.

**Email: weiwei.lei@deakin.edu.au*

Modern society and daily life are facing a severe challenge from the lack of clean water and electricity. However, the technologies of generations of clean water and electrical energy are currently independent.[1,2] Therefore, exploring an integrated solution for the co-generation of clean water and electricity is essential. Due to its low carbon footprint, interfacial solar-driven water evaporation has been a promising green and sustainable solution for alleviating the global water shortage problem.[3] Especially, the water evaporation can result in a continuous, directional capillary water flow from the bulk water to the evaporation interface, which will trigger the hydrovoltaic effect and produce power energy. These features of the solar-driven water evaporation system provide a potential platform to simultaneously generate steam and electricity by using solar energy.

Recently, two dimensional (2D) based nanomaterials, including the graphene-family, BN, exfoliated dichalcogenides, layered metal oxides, zeolites, and metal–organic framework (MOF) nanosheets, MXene, offer an exciting opportunity for developing a new family of advanced nanomaterials and membranes featuring unique properties including super thermal stabilities, high resistance to oxidation, excellent chemical inertness, and electrical insulation.[4-7] Here, we have developed a series of functionalized 2D nanomaterials such as graphene, BN, MoS_2, MXene, metal nitrides with unprecedented 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 storage, and broadband (UV-visible-Infrared) light absorption and excellent photothermal conversion efficiency for freshwater generation. [8-17]

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IL45 Granular hydrogels for promoting tissue regeneration

Haiyan Li, [1, 2]*, Zhijie Ma[2], Wei Song[3], Dan He[2], Xing Zhang[2], Yaohua He[3]

[1]*Chemical and Environmental Engineering, School of Engineering, RMIT University*
[2]*School of Biomedical Engineering, Shanghai Jiao Tong University*
[3]*Department of Orthopaedics, the Sixth People's Hospital, Shanghai Jiao Tong University*
**Email: haiyan.li4@rmit.edu.au*

Hydrogels have proven useful in regenerative medicine. However, conventional hydrogels inherently have nanoporous structure, which limit mass transport of key biomolecules and restrict the behaviour of cells and infiltration of surrounding tissue and cells. Granular hydrogels show great promise in tackling the problems of the conventional nanoporous hydrogels. Additionally, to closely recapitulate the inherent healing cascades, sequential delivery strategies are urgently need for enhancing various kinds of tissue regeneration.

Here, we reported novel granular injectable microporous hydrogels for promoting wound healing and articular cartilage regeneration. The hydrogels were designed and fabricated with widely used biomaterials and encapsulated additional bioactive ingredients for stimulating different stages of wound healing. A bioactive macroporous self-healable hydrogel by assembling methacrylated hyaluronic acid (MeHA) and 3-aminophenylboronic acid modified sodium alginate (SABA) microgels. The obtained microporous hydrogels have larger pore size than nanoporous hydrogels, which facilitated cell infiltration, viability and proliferation. Meanwhile, the macroporous hydrogels had good self-healing abilities with the formation of dynamic B-O bonds. Furthermore, with the bioactivity of BG, the hydrogels could induce cell migration and ingrowth of cells and blood vessels.

We also designed a novel granular hydrogel for articular cartilage regeneration. The macroporous hydrogel was fabricated by assembling sodium alginate (SA) and hyaluronic acid (HA) (SA/HA) micro-fibres (μ-fibres) into microporous hydrogels. The exosomes derived from NR8383 cells activated by lipopolysaccharides (LPS) and stimulated with bioglass (BG) ion extracts (LPS/BG-exo) could be released from the hydrogel to inflammation homeostasis and recruit BMMSCs. Meanwhile, poly (lactic-co-glycolic acid) (PLGA) microspheres containing kartogenin (KGN) ($PLGA_{KGN}$) were encapsulated within the hydrogel for inducing the chondrogenic differentiation of recruited BMMSCs when KGN is released after the LPS/BG-exo. The obtained macro-porous SA/HAexo-$PLGA_{KGN}$ hydrogel can enhance the cartilage regeneration in a rat cartilage defect model.

In conclusion, granular injectable hydrogels have great applications in tissue regeneration.

IL46 Reduce energy loss in water electrolysis

Wenxian Li[1]*, Riyue Ge[2]
[1]*School of Materials Science and Engineering & UNSW Materials & Manufacturing Futures Institute, University of New South Wales, Sydney, New South Wales 2052, Australia*
[2]*School of Materials Science and Engineering, Shanghai University, Shanghai 200444, China*
**Email: wenxian.li1@unsw.edu.au*

Overpotential in water electrolysis refers to the extra potential that exceeds the theoretical potential of 1.23 V, which is caused by energy losses in the circuit, the energy barrier of charge transfer, and unfavourable mass transport. Transition metal compound nanoparticles are frequently used as low-cost catalysts for HER and OER to increase active and specific surface areas for good electron transfer and mass transport. However, because of their poor conductivity and low mass transport for agglomeration, nanosized transition metal compounds are challenged by poor inter- and intra-particle charge transfer, which induces an overpotential to consume >80% extra energy for water splitting. To tackle the circuit energy consumption, we developed an ion-bridging method to optimize the charge transfer behaviour between two phases of nanocomposite.[1-3] The method is suitable for fabricating nanomaterials with low overpotential and large specific surface area. We also developed confined growth of hierarchical nanostructures to fabricate MoP catalysts for HER to improve the mass transport in water splitting.[4] We also fabricated HER and OER catalysts includes ion-induced architecture and MOF templated construction which has been verified in the fabrication of Ni_xCo_yP/Co_2P heterostructure,[5] trimetallic CoNiFe carbonate hydroxide micro-flowers,[6] Ni/Mo_2C hybrids anchored on nitrogen-doped carbon nanosheets,[7] and transition Metal-Mo_2C heterostructure.[8]

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IL47 Thermostable 1T MoS_2 by spontaneous intercalation of Cu single atoms and the enhanced water splitting performance

Mengyao Li [1*]

[1] *School of Materials Science and Engineering, University of New South Wales, Sydney, NSW 2052, Australia*

**Email: mengyao.li1@unsw.edu.au*

We report a simple strategy to fabricate Cu single atoms (SAs) layer-intercalated MoS_2 only by stirring Cu metals with MoS_2 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 MoS_2. Notably, the 1T-metallic phase after Cu intercalation could be maintained even at 800 ^{o}C, breaking the record to the best of our knowledge. Besides, the as-prepared MoS_2/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-MoS_2 may make it suitable catalyst applied at high temperature, such as ammonia synthesis and CO_2 conversion. [1]

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IL48 Developing high-voltage spinel cathodes for high-energy-density lithium-ion batteries

Gemeng Liang [1]*, Zaiping Guo [1]

[1] School of Chemical Engineering, The University of Adelaide
**Email: gemeng.liang@adelaide.edu.au*

Lithium-ion batteries (LIBs) with high energy densities are crucial to meet the increasing power demands of developing technologies.[1] The performance limitation in existing battery technology is cathode material, therefore stimulating extensive research efforts around the world to explore new high-performance cathode materials. Spinel $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) is considered one of the most promising electrode candidates for next-generation LIBs owing to its high operating voltage (~4.7 V vs Li), high energy density (650 Wh kg^{-1}), and low fabrication cost.[2] However, its structural instability during charge and discharge leads to rapid capacity decay, and limits its practical application. We have successfully stabilized the spinel structure by elemental doping via site-specific structural engineering at the *Fd*-3*m* 8*a*, 16*c* and 16*d* Wyckoff sites.[3,4] Additionally, a novel and strong 4*s*-2*p* orbital interaction has also been introduced into the spinel oxide material,[5] which differs from the conventional and weak 3*d*-2*p* chemical interactions in the transition metal oxide cathodes, and contributes to the significantly enhanced structural stability. It is expected that useful insights could be obtained from our work to develop stable and competitive cathode materials for next-generation high-energy-density LIBs.

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IL49 Interfacial engineering of glassy metal-organic framework composites

Rijia Lin,[1] Vicki Chen,[2] Lianzhou Wang,[1,3] Jingwei Hou[1]*

[1] School of Chemical Engineering, The University of Queensland, St Lucia, QLD, 4072 Australia
[2] University of Technology Sydney, 15 Broadway, Ultimo, NSW 2007, Australia
[3]Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St Lucia, QLD, 4072 Australia
**Email: Jingwei.hou@uq.edu.au*

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

This work will introduce our studies in glassy MOF composite materials for membrane separation and electrochemical applications, focusing on optimizing the composite interface. We developed a MOF glass mixed matrix membrane by *in situ* melting of ZIF-62(Zn) within the polyimide matrix.[3] The *in situ* melting of glassy MOF effectively healed the defects at the MOF-polymer interface, which led to a 57% increase in CO_2/N_2 selectivity for the composite membrane compared to the pure polymeric counterpart. Utilising the reactivity of MOF liquids, a bimetallic MOF glass hybrid was prepared by melting the ZIF-62(Co) together with an adsorbed ferric coordination complex.[4] The reactive ZIF-62(Co) liquid facilitates the formation of coordinative bonds between Fe and imidazolate ligands. The presence of bi-metal ions within the framework significantly improved the catalytic oxygen evolution reaction (OER) performance of the MOF glass. Moreover, we introduced a rapid mechanochemical technique to produce MOF glass coatings on carbon cloth for fabricating larger area electrodes.[5]

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IL50 Structural studies of solid-state ionic conductors at the limits of diffraction and beyond

Chris Ling[1]

[1] School of Chemistry, The University of Sydney
**Email: chris.ling@sydney.edu.au*

The structures of solid-state ionic conductors are a compromise between long-range (and hence long-term) lattice stability and short-range coordinative flexibility. To rationally design improved versions for applications such as fuel cells and batteries, we need to understand how this compromise is reached. Diffraction methods alone are inadequate – whether using X-rays or neutrons, *ex situ* or *operando*, conventional crystallography or total scattering analysis – because of their dynamic nature. The time-averaged structure is not the whole story. In this talk I will show how we use experimental X-ray and neutron spectroscopy, and computational structure and dynamics calculations, to supplement diffraction when studying solid-state oxide, proton and lithium ionic conductors. We can then validate the insights gained by making targeted chemical modifications and testing their effects on structure and functional physical properties.

IL51 Novel 2D nanomaterials for thermal management and energy storage

Zhiyu Wang[1], Dan Liu[1]*
[1]*Institute for Frontier Materials, Deakin University, Waurn Ponds Campus, Locked Bag 20000, Victoria 3220, Australia*
Email: dan.liu@deakin.edu.au

With the development of technology in civilian and military, high-power density electronic devices are more frequently used than before, resulting in excessive thermal energy accumulation. Therefore, the development of nanomaterials with anisotropic thermal transport properties has attracted increasing attention for thermal management applications, such as coatings in electronics and heat sinks. An ideal candidate should be electrically insulating and have thermal conductivity in-plane significantly greater than through-plane. Two-dimensional (2D) nanomaterials such as graphene and black phosphorus, both of which possess highly anisotropic thermal conductivity, have recently provided a new platform for addressing heat dissipation in devices. However, it is difficult to employ either in thermal management or build components owing to their electrical conductivity and fast oxidation of phosphorus.

Boron nitride (BN) nanosheets offer a high thermal conductivity. In contrast with other conductive and semiconducting 2D materials, BN nanosheets are electrically insulating, which suggest utility in thermal management applications in electronics.[1] Here, we report free-standing BN nanosheets membrane and their composite films with unique combination of properties including flexibility and toughness, anisotropic thermal conductivity, and fire resistance, which exhibit highly potential applications in high-performance flexible electrically insulating substrates, thermal energy regulation, energy storage and fire-resistance coatings.[2-8]

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IL52 Atomically dispersed Silver-Cobalt dual-metal sites synergistically promoting photocatalytic hydrogen evolution

Yazi Liu[1], Yue Sun[1], En Zhao[2], Shaogui Yang[1], Huan He[1]*, Zupeng Chen[2]*, Shaobin Wang[3]

[1] *School of Environment, Nanjing Normal University, Nanjing, 210023, P.R. China*
[2] *Jiangsu Co-Innovation Center of Efficient Processing and Utilization of Forest Resources, International Innovation Center for Forest Chemicals and MaterialsNanjing Forestry University, Nanjing, 210037, P.R. China*
[3] *School of Chemical Engineering, The University of Adelaide, Adelaide, SA 5005, Australia*

** Email: huanhe@njnu.edu.cn (H. He); czp@njfu.edu.cn (Z. Chen)*

Regulating the coordination environment of single-atom sites is of high necessity to promote the catalytic performances of the photocatalysts. Herein, we report the preparation of atomically dispersed Co-Ag dual-metal sites anchored on P-doped carbon nitride (Co_1Ag_1-PCN) via supramolecular and solvothermal approaches, which demonstrates desirable performance for photocatalytic H_2 evolution from water splitting. The optimal Co_1Ag_1-PCN catalyst achieves a remarkable hydrogen production rate of 1190 μmol g^{-1} h^{-1} with an apparent quantum yield (AQY) of 1.49% at 365 nm, superior to most of the newly reported metal-N-coordinated photocatalysts. Systematic experimental characterizations and density functional theoretic studies attribute the enhanced photocatalytic activity to the synergistic effect of Co-Ag dual sites with exclusive coordination configuration of Co-N_6 and Ag-N_2C_2, which enhances the charge density and promotes oriented electrons transport to the metal centers with reduced free energy barriers by facilitating the formation of H* intermediates as the key step in hydrogen evolution. This study reveals a versatile strategy to tailor the electronic structures of dual-metal sites with synergies by engineering the neighboring coordination environment.

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IL53 Multiscale structural parameters affecting antiferroelectric-ferroelectric phase transition

Teng Lu[1], **David Cortie**[2], **Dehong Yu**[2], **Yun Liu**[1]

[1] *Research School of Chemistry, Australian National University, Canberra, Australian Capital Territory 2601, Australia.*
[2] *Australia Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, New South Wales 2234, Australia*

**Email: Teng.Lu@anu.edu.au*

Polar functional materials, such as ferroelectrics (FEs), play a vital role in modern electronic devices like capacitors, sensors, and FeRAM. In addition to FE materials, antiferroelectric (AFE) materials with the antiparallel-aligned polar order have recently raised tremendous research interest due to their promising energy conversion and storage applications. These applications mainly stem from the unique structural transitions triggered by external stimuli like electric fields (E-field), temperature, and mechanical force.[1] Consequently, it becomes pressing to unveil the structure parameters affecting the phase transitions. This study comprehensively investigates the structure-property relationship in the prototype $PbZrO_3$- and $AgNbO_3$-based antiferroelectric materials using complementary structural analytical techniques.[2,3] It elaborates that structures at different lengths from the micro (domain alignment and crystallographic texture) to nano (correlated atomic displacements and octahedral tilting) scales impact the critical E-field required for triggering the AFE-FE phase transition. Moreover, it demonstrates that these critical structural parameters, which reflect the energy barrier between AFE and FE phases, can be modified through chemical compositions, external E-field, and temperature. The results illustrate that manipulating multiscale structure parameters allows for tuning AFE material properties. Importantly, these parameters can be adjusted not only through chemical compositions and synthesis conditions but also controlled by the history of applied E-field and temperature. Therefore, this study provides flexible structural parameters for tailoring the physical properties of AFE materials, offering new strategies to enhance the performance of AFE materials and devices.

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IL54 Design and characterisation of one-dimensional organic molecular materials

Jennifer MacLeod[1]*

[1] *School of Chemistry and Physics and Centre for Materials Science, Queensland University of Technology (QUT), Brisbane, Australia*
**Email:* *jennifer.macleod@qut.edu.au*

Bottom-up approaches hold promise for synthesising bespoke nanomaterials. Using suitably-chosen organic molecular building blocks, we can target the structure and function of the product materials.[1] Constructing these materials on a surface provides further control of the structure: the surface enforces planarity, provides an epitaxial template, and can also modify the deposited molecules by acting as a catalyst and by donating adatoms. The variety of available molecular building blocks and surfaces provides access to a near-infinite range of 1D and 2D structures.

In this talk, I will focus on our recent work in using small molecule precursors to synthesize one-dimensional nanomaterials through on-surface reactions, through both surface-catalysed and electron-induced reactions.[2] Using these approaches, we have investigated the on-surface reaction and coupling of a range of small aromatic molecules on transition metal surfaces. Using key surface science techniques (photoelectron spectroscopy, inverse photoelectron spectroscopy, scanning tunneling microscopy, density functional theory) we perform detailed investigations into the reaction process and products, providing insight into the formation of these architectures, and demonstrating some of the novel characteristics of the materials formed through these processes and elucidating their structure/function relationships and suitability for future applications.

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IL55 Design of solid-electrolyte interphase for emerging aqueous zinc metal batteries

Jianfeng Mao[1]*

[1]*School of Chemical Engineering, The University of Adelaide, Adelaide, SA, 5005 Australia*

Email: jiafneng.mao@adelaide.edu.au

The development of advanced energy storage systems is urgent to transform our society into one based on renewable energy resources, in which rechargeable batteries are one of the most promising approaches but remains to be solved. Aqueous Zn metal batteries promise high capacity, low cost, high safety, and sustainability for large scale energy storage. Their Zn metal anode suffers, however, from side reactions and dendrite growth that occur at the Zn-electrolyte interface, and these considerations limit their full potential [1]. Regulating the electrolyte formulation for in-situ construction of highly Zn^{2+}-conductive solid-electrolyte interphase is a promising approach to handling these interface-related issues. In this talk, I will introduce our recent work on rational electrolyte design and interphase engineering for Zn metal batteries [2-6] and will discuss the issues and opportunities for building better batteries.

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IL56 Caveman's quantum computer: ferromagnetic nanographene synthesis in flames

Jacob Martin[1]*

[1]*Department of Physics and Astronomy, Curtin University, Bentley, Perth, 6845, WA, Australia*

Email: jacob.w.martin@curtin.edu.au

Nanographenes have been touted as a possible source for quantum computing bits. Aromatic molecules have been prepared that possess a triplet diradical or ferromagnetic ground state. In this work, we used non-contact AFM and quantum chemistry calculations to find and understand flame generated localised pi-radical states that enabled triplet diradicals to be stabilised. This provides a possible route to the synthesis of nanographenes and a better understanding of the role of pi-edge states in stabilising high-spin nanographenes.

IL57 BTEX from Lignin using a Novel Molybdenum Carbo-nitride@Titanium Nitride Catalyst

Matthew Lui[1] , Alexander Yuen[2] , Stuart Bartlett[3] , Anthony Masters[2] ,* Thomas Maschmeyer[2]
[1]*Department of Chemistry, Hong Kong Baptist University, Hong Kong*
[2] *School of Chemistry, The University of Sydney, Sydney, 2006, Australia*
[3] *Diamond Light Source, Harwell Science & Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK*
**Email: anthony.masters@sydney.edu.au*

This study unveils the key structural features and compositional aspects of several molybdenum hemicarbide-based catalysts using a combination of synchrotron techniques, X-ray diffraction and elemental mapping in conjunction with electron microscopy [1] as well as their catalytic performance in the conversion of lignin to BTX using supercritical ethanol and base. [2]
The composite was shown to be more effective than either Mo_2C or Mo_2N for the hydrodeoxygenation of lignin to single-ring arenes in supercritical ethanol. EXAFS experiments at 330 °C, under a stream of ethanol vapor to approximate in situ conditions, elucidate the importance of the interaction of the titanium nitride support with the molybdenum carbo-nitride phase. The TiN and Mo_2C phases are intimately mixed as revealed by EXAFS EDAX, TEM, etc.. Supported Mo_2C catalysts were prepared and employed to depolymerize and deoxygenate waste lignins to aromatics in supercritical ethanol. TiN appears be a particularly beneficial support material. Depolymerization at 330 °C gave a higher yield and selectivity for arenes than at 280 °C. Base is essential for efficient substrate conversion: the basic constituents inherent in waste lignins are suitable, as is added sodium hydroxide. Without base, depolymerization is poor, the yield of aromatics is very low, and substrate defunctionalisation does not occur. A significant proportion of aromatic products is formed from supercritical ethanol itself, including benzene, which is likely to be present in all catalytic runs due to ethanol aromatization. Hence the total arene content produced is actually higher than has been widely reported. Catalytic cracking of ethanol leads to C1-units, which add to reaction intermediates to give aromatics containing odd numbers of carbons (e.g. toluene).
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IL58 Designing thermal energy storage for industrial applications

Karolina Matuszek,[1]*

[1] *School of Chemistry, Monash University, Clayton, Australia*
**Email: karolina.matuszek@monash.edu*

Renewable energy has the ultimate capacity to address the world's energy supply challenges and environmental concerns. Implementation of solar and wind energy-harvesting technologies has rapidly expanded world-wide, at both grid-scale and domestic levels. Their utilization, however, is strongly constrained due to the lack of efficient and economical energy storage solutions, which are pivotal in bridging the gap between demand fluctuations and supply intermittency. In this context thermal energy storage technologies (thermal batteries), which store energy in the form of heat, can offer distinct advantages, including high energy storage capacity, low cost, reliability, and easy scalability.[1] Among them Carnot Battery is an interesting concept that integrates thermal storage with heat pump and organic Rankine cycle engine. This configuration enables to store input of electrical energy, from wind or solar, in the form of heat and in the discharge mode to deliver electricity and lower grade heat as depicted in Figure 1.[2] Currently demonstrated power-to-power round trip efficiencies are reaching 72 %. Essential for maximizing the potential of this technology is the selection of an appropriate thermal energy storage material. Such material should not only exhibit a high thermal energy storage capacity and suitable operational temperature but there are other crucial factors to be considered. This talk will discuss these aspects from techno-economic assessment, sustainability to life cycle analysis.

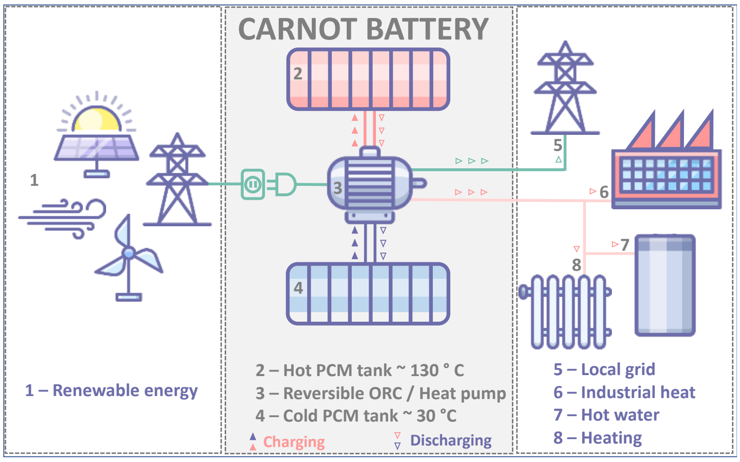

Figure 1. Schematic of Carnot Battery with integrated thermal energy storage system.[2]

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IL59 Insights into metal transport in ore-forming processes through molecular simulations

Yuan Mei[1]*, Weihua Liu[1], Joël Brugger[2]

[1] CSIRO Mineral Resources, Kensington, WA 6151 Australia
[2] School of Earth, Atmosphere and the Environment, Monash University, Clayton, VIC 3800, Australia
**Email: yuan.mei@csiro.au*

The formation of mineral deposits is heavily influenced by the interaction between minerals and fluids in the lithosphere and hydrosphere. Fluids with complex chemical compositions at high pressure and temperature transport metals in ore-forming systems. The hydration and complexation of metals in hydrothermal fluids play a crucial role in dictating the mobility of elements in the Earth's crust, leading to the formation of ore deposits that are mined for valuable resources of base, precious and critical minerals. To gain a molecular-level understanding of the chemical processes responsible for the formation of the ore deposits, we have integrated computational chemistry techniques with synchrotron-based X-ray absorption spectroscopy experiments. This approach enables us to examine the thermodynamics of metal and ligands in fluids that form ore deposits.

In particular, the ab-initio molecular dynamics simulations, which describe inter-atomic interactions through quantum mechanics, offer a method to investigate the nature and stability of metal complexes under conditions that are beyond experimental practicality. In the past decade, we have used this approach to examine the complexation of Cu, Au, Zn, Pd, Pb, Y, La and Mo in chloride- and hydrosulfide-rich aqueous fluids at extreme temperatures and pressures, as well as the behaviour of Cu and Au in low-density vapours and in CO2-rich fluids. Encouragingly, the results from the simulations match experimental results, demonstrating that ab-initio MD simulations can provide quantitative energetic properties for metal complexation and hydration under hydrothermal conditions in fluids that are outside of experimental boundaries. In this presentation, I will provide an overview of our recent investigations and showcase the potential of this integrated approach in enhancing our understanding of the formation of mineral deposits.

IL60 Modeling and methods for the characterisation of Olivine/water interfaces for CO_2 sequestration.

Izaac Mitchell,[1]* Raffaella Demichelis[1]

[1] School of Molecular and Life Sciences (MLS), Curtin University
**Email: izaac.mitchell@curtin.edu.au*

CO_2 driven climate change is one of the great, if not greatest, global challenges in modern society. The need to limit CO_2 emissions is in contrast with the need to increase energy production due to the simultaneous global population growth and global improvement of life quality. Potential ways to compensate for CO_2 emissions are CO_2 geosequestration and carbon neutral fuel cycles. Here, olivine minerals ($XYSiO_4$, with X and Y being bivalent cations) and other silicates are interesting candidates. In fact, olivine can naturally react with water and CO_2 to produce methane in some conditions[1] or can naturally sequester CO_2 through dissolution of the silicate phase and reprecipitation of carbonate minerals in others.[2] Unfortunately, these processes occur in complex geochemical and geophysical environments, limiting the experimental capability to define chemical reactions accurately. Computational methods have the potential to bridge this gap of knowledge; however, modelling the reactivity at a liquid-solid interface is still a methodological challenge due to having to explore large time and size scales at a highly accurate level of theory. This work presents the application of several available methodologies to investigate the forsterite (Mg_2SiO_4)/water interface and discusses possible avenues for modeling these complex systems.

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IL61 Simulating molecular flow

Stephen Sanderson[1]*, Amy Geddes[1,2], Shern Tee[1,3], Emily Kahl[1], Marco de la Pierre[3], Debra J. Searles[1,4]

[1] *Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St Lucia, QLD, 4072, Australia*
[2] *Pawsey Supercomputing Centre, Kensington, WA, 6151, Australia*
[3] *School of Environment and Science, Griffith University, Nathan, QLD, 4111, Australia*
[4] *School of Chemistry and Molecular Biosciences, The University of Queensland, St Lucia, QLD, 4072, Australia*
**Email: stephen.sanderson@uq.edu.au*

Molecular dynamics (MD) simulations provide various methods for nanoscale flow modelling. Some are applicable to confined flows, while others model flow in the bulk. Although most methods appear conceptually simple, they are complicated by the need for a thermostat to prevent infinite heating. From this, a number of subtleties arise which may cause incorrect results, especially at high flow rates. This is particularly true when modelling bulk molecular flow, where all atom velocities include some streaming component which is not thermal (and should therefore not be thermostatted), and the streaming velocities are non-trivial due to rotational motion of molecules.

This talk gives an overview of key considerations when simulating flow, before focusing on the case of bulk molecular flow. As part of a Pawsey Centre for Extreme Scale Readiness (PaCER) project, we are extending the functionality of the popular MD package LAMMPS to allow for bulk molecular flow modelling using well-established, yet not widely implemented, algorithms which aim to avoid spurious effects at high flow rates. An outline is given of the applicability and key details of these algorithms, along with some preliminary results.

IL62 Piezofiber to smart textiles: processing and challenges

Fatemeh Mokhtari*, Russell Varley

[1]*Carbon Nexus, Institute for Frontier Materials, Deakin University, Victoria 3216, Australia*
**Email: fatemeh.mokhtari@deakin.edu.au*

Recent developments in miniaturized electronic devices with sophisticated computational capabilities and remarkably low-power communication technologies have led to a trend toward powering these devices with long cycle life, high energy efficiency, fast and cost-effective production, and lightweight power sources. The integration of piezoelectric materials and novel fabrication techniques with conventional textile processes has given rise to the emergence of a wearable technology field, which can serve multiple applications, such as structural health monitoring systems, self-powered wireless sensors, and cost-effective energy harvesting from body movements.[1] Organic piezoelectric materials, such as poly(vinylidene fluoride) PVDF, exhibit distinct features of chemical stability and flexibility, facilitating the fabrication process of fiber-based devices. However, polymers have limitations in terms of a high electric field and low dielectric constant during the poling process.

Inorganic piezoelectric materials, such as piezo ceramics, possess outstanding piezoelectric properties but cannot be easily melted or solubilized in a solvent for processing into fiber forms. They must be spun from precursor materials and subsequently thermally treated for densification and sintering. These delicate processes require careful control to optimize the piezoelectric properties of the fibers.[2]

In light of these challenges, we have explored novel approaches to develop high-performance piezo composite, all fiber-based energy harvesting devices as the next generation of wearable energy generators and sensors. These devices offer key advantages for use in human garments, including flexibility, stretchability, lightweight design, and ideal interface options between the environment, electronic devices, and the human body. Various textile designs, ranging from melt-spinning and knitting to braiding and weaving, have been developed with capabilities for low-cost, high-speed production and exceptional performance.

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IL63 Characterization and material growth of two-dimensional transition metal dichalcogenides

Hieu T. Nguyen

College of Engineering, Computing and Cybernetics, The Australian National University
Email: hieu.nguyen@anu.edu.au

Atomically thin two-dimensional (2D) transition metal dichalcogenides (TMDs) exhibit novel and promising properties for future optoelectronics. These properties include atomically thin flexibility and lightweight, excellent optoelectronic properties, courtesy of the quantum-confinement effects in their monolayers, which improve their absorption efficiency. Additionally, their surfaces naturally undergo passivation, making it possible to construct various vertical heterostructures without encountering lattice mismatches. Despite intensive and extensive studies on this class of materials over the past decade, some important properties are still not thoroughly investigated. Moreover, it remains challenging to grow uniform, high-quality, and large-area 2D TMD monolayers.

In this presentation, I will present my team's latest advances in the characterization and material growth of 2D TMDs. Particularly, I will introduce a method to quantify the Quasi-Fermi Level splitting of various 2D TMD materials under illumination, which is equivalent to the maximum open circuit voltage of an ideal solar cell when that material is used for solar cell fabrication. Subsequently, I will discuss the effects of twist angles on the optical properties of p-n-like MoS_2/WS_2 heterobilayers, including light emission and absorption, minority carrier lifetime, and minority carrier diffusion. Finally, I will present some of our results in the material growth of large-scale, high-quality 2D TMD monolayers, reaching dimensions in the millimeter range.

IL64 What can we learn about cvd and nanomaterial growth using computational approaches?

Alister J. Page[1]*

[1] *Discipline of Chemistry, University of Newcastle, Callaghan 2308, NSW Australia*
**Email:* alister.page@newcastle.edu.au

Over the last few decades, catalytic chemical vapor deposition (CVD) has matured as a synthetic technique for producing many low-dimensional inorganic nanomaterials, such as carbon nanotubes (CNTs), graphene, boron nitrides and transition metal dichalcogenides. van der Waals heterostructures comprising these 1D and 2D allotropes have also been recently developed. During this time, Computational approaches have played a critical role in developing our understanding of the structure, properties and growth of these materials. In this talk, I will summarise our own recent contributions to this field, and will discuss how molecular dynamics and quantum chemistry help us understand the chemistry of CVD nanomaterial growth [1,2], nucleation mechanisms of 1D and 2D inorganic nanomaterials [3] and heterostructure stability [4]. I will also discuss our work employing machine learning and graph-neural network approaches for identifying improved heterogeneous catalytic interfaces for CVD nanomaterial growth [5].

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IL65 Site-specific Doping Strategy for Better-performance Energy Materials: A Root-cause Analysis Using Neutron and X-ray Scattering

Wei Kong Pang[1]*

[1] *Institute for Superconducting and Electronic Materials, University of Wollongong, North Wollongong, Australia.*
**Email: wkpang@uow.edu.au*

Lithium-ion batteries (LIBs) have become a cornerstone of our modern daily life and were recognized with the prestigious 2019 Nobel Prize in Chemistry. The symmetrical structure of an electrode structure forms a matrix of scaffold arrays, facilitating a specific route for the charge carriers to diffuse in and out. Among promising cathode candidates for next-generation high-energy-density LIBs, disordered spinel $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) [1-3] and lithium-rich layered oxide $Li_{1+x}TMO_2$ (TM = Mn, Ni, etc.) [4] have garnered considerable attention due to their unique Fd-3m cubic space group and R-3m/C2/c intergrown structure, resulting in distinct 3D and 2D lithium-ion diffusion pathways and varied electrochemical performance. In this work, we leverage expertise in energy storage, crystallography, materials science, and advanced characterization techniques to engineer the crystal structure of these electrodes with precision. Our goal is to address the root causes of instability by targeting specific crystallographic sites through a fundamental structure/function relationship approach. The aid of neutron and X-ray scattering techniques enables us to achieve exceptional durability and phenomenal performance for intercalation-type electrodes. This presentation showcases the effectiveness of crystallographic-site-specific doping, and the uses of neutron and X-ray scattering, and sheds light on novel approaches for enhancing the electrochemical performance of LIBs. This work opens new horizons in the quest for advanced energy storage systems and paves the way for the design and development of even more efficient and long-lasting batteries.

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IL66 Engineered living and dead materials: from 3d printable enzyme plastics to living bacterial microreactors

Adam Perriman [1*]

[1] *Research School of Chemistry, Australian National University, Building 137, Sullivans Creek Rd, Acton, ACT 2601 Canberra, Australia*
**Email: Adam.Perriman@anu.edu.au*

Engineered living and dead materials present an exciting opportunity to integrate and scale outputs from synthetic biology. Such materials are currently being developed for a wide variety of applications, which range from gut microbiome re-engineering to fungal-bacterial composite building materials. Ideally, the biological component should interface with and modulate the bulk structure and function of material, by driving assembly or chemical processes from the nano to the macro length scales. Accordingly, we present recent and ongoing research on the development of smart highly fabricable composite bionanomaterials and engineered living materials with tuneable emergent properties. Specifically, we describe the development of enzymatically-active melts[1], membranes[2, 3] and plastics[4], with robust high fidelity structures, a new class of bioink comprising an oxidoreductase-mediated interpenetrating network (IDE) gel with thermoresponsive shape changing properties[5] and a 3D bioprinted living bacterial microreactor that is capable of detoxifying organophosphates under flow.

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IL67 Direct measurement of structural change with amorphous solidification from static speckle scattering

Charlotte Petersen[1]*, Peter Harrowell[2]

[1] School of Chemistry, University of Melbourne, Melbourne, Victoria 3010 Australia
[2] School of Chemistry, University of Sydney, Sydney, New South Wales 2006 Australia
**Email: charlotte.petersen@unimelb.edu.au*

Scattering experiments that measure the static structure factor are the standard structural determination tool for crystalline materials. However, their utility is limited for amorphous materials, where the lack of periodic order means structural signatures become washed out; Only average structural information can typically be obtained. In addition to these measurement difficulties, we lack a complete theory to predict the rigid behaviour of glass from its amorphous microscopic structure.

Recent progress has connected the presence of localised soft normal modes to the dynamics of glass [1,2]. Building on this success, the capacity of a configuration to restrain particle motion has been formalised as a structural order parameter that characterises the solidification of a liquid into an amorphous solid on cooling [3]. However, this quantity cannot be measured in experiments. Here, we demonstrate that the Debye-Waller factor, which quantifies particle vibrations from the static structure factor, is a suitable experimentally accessible structural order parameter to characterise solidification. Despite the weak temperature dependence of the spherically averaged static structure factor, we find that the Debye-Waller factor of a simulated glass extracted from the speckle scattering at individual wavevectors shows a strong temperature dependence. We also extract from the speckle intensities a quantity proportional to the variance of the local restraint, i.e. a direct measure of the amplitude of structural heterogeneity.

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IL68 Bridging the gap between atomistic simulations and experimental thermodynamics in geochemical systems

A. Silvestri, B. I Armstrong, J. D Gale and Paolo Raiteri[1]

[1] *School of Molecular and Life Sciences, Curtin University, Perth WA*
**Email: p.raiteri@curtin.edu.au*

The ubiquitous integration of computer simulations in scientific and engineering research has allowed significant advances in our understanding of complex phenomena. Today, atomistic simulations of geochemical systems offer powerful insights at the nanoscale. However, despite their increasing accuracy, bridging the gap between simulation results and experimental data remains a significant challenge. One complicating aspect of this endeavour lies in the proper definition of standard reference states for the simulations. While experimental data are typically referred to a well-defined thermodynamic state (1 mol/L and 1 bar), the same cannot always be said for atomistic simulations. In fact, each simulation has its unique reference state, which depends upon factors such as system size, use of restraints/constraints, and ensemble choice. This difference between the reference states used poses a substantial obstacle when attempting to compare simulation outcomes with both experimental observations and results from other simulations.

In this presentation, I will discuss how we can reconcile the ion adsorption free energies of minerals computed with different methods, and with the predicted solubilities of the solids. This requires a careful design of the simulations and the inclusion of all the appropriate contributions to refer the results to the thermodynamic standard state. In order to illustrate this approach, I will use two of the most well-studied minerals, namely halite and calcite.

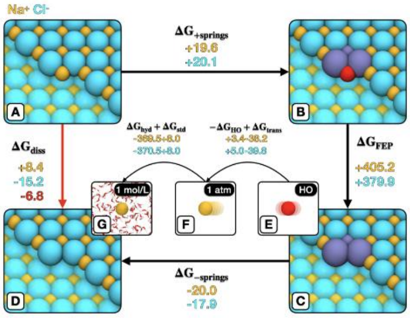

Figure 1. Thermodynamic cycle for the determination of the free energy of dissolution of NaCl. [1]

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IL69 Solid-state nuclear magnetic resonance spectroscopy for materials characterization

Aditya Rawal[1]

[1]NMR Facility, Mark Wainwright Analytical Centre, UNSW Sydney
**Email: a.rawal@unsw.edu.au*

Nuclear magnetic resonance (NMR) comes in three flavors. The well known MRI, which has revolutionized medical imaging, solution state NMR, which is crucial for determination of chemical structures and the lesser known solid-state NMR spectroscopy which is applied to materials and biomolecular systems. Complementary to diffraction and microscopy techniques, NMR enables an in-depth analysis of the molecular level structure of complex materials. In favorable cases, it is possible to provide a detailed molecular structure-property relationship based on the NMR data.

In the present talk, I will highlight how solid-state NMR provides a platform for materials characterization of diverse materials, with applications in pharmaceutical science, civil engineering, energy storage, nano-materials and biomaterials. In all cases, we see how NMR is able to provide qualitative and quantitative insights into materials structure even in the absence of any long range. It is hoped that the presentation will encourage further uptake of this powerful technique within the materials community.

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IL70 Understanding functional porous materials with low-field nmr relaxation

Neil Robinson[1]*

[1] *Department of Chemical Engineering, The University of Western Australia,*
Perth WA 6009, Australia
**Email: neil.robinson@uwa.edu.au*

Functional porous materials underpin a vast range of critical chemical processes, ranging from fuel storage and sustainable building material formulation, to pollution abatement and the production of materials and chemicals from renewable resources. The underlying chemical and physical processes associated with such applications are a direct result of the interactions of these porous structures with fluids (gases, and/or liquids) via their encapsulation, surface adhesion, and/or chemical reaction. Despite their ubiquity and high industrial and socioeconomic importance, however, notable knowledge gaps remain regarding the properties of fluids confined within such materials. Indeed, the characterisation of chemical reaction and interaction phenomena occurring within the void spaces of optically opaque porous structures remains one of the most significant challenges in physical science and engineering, requiring measurement approaches with the ability to reliability discriminate between molecules interacting with the interface(s) of interest, and the surrounding solid and fluid components. This talk will provide an introductory overview of the application of nuclear magnetic resonance (NMR) relaxation measurements to such problems, which provide a versatile, non-invasive and chemically selective approach with which to characterise fluid interactions within porous solids, and may be implemented under operando pressure and temperature conditions of direct relevance to industrial chemical processes. Such measurements have been employed by the rock physics and hydrocarbon recovery community for over five decades, but their application to well-defined functional porous materials has until now been extremely limited. Correspondingly, this talk will highlight recent applications of nuclear spin relaxation to materials of relevance to catalysis [1-3], gas process engineering [4] and construction [5,6].

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IL71 Simulating molecular flow

Stephen Sanderson[1]*, Amy Geddes[1,2], Shern Tee[1,3], Emily Kahl[1], Marco de la Pierre[3], Debra J. Searles[1,4]

[1] Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St Lucia, QLD, 4072, Australia
[2] Pawsey Supercomputing Centre, Kensington, WA, 6151, Australia
[3] School of Environment and Science, Griffith University, Nathan, QLD, 4111, Australia
[4] School of Chemistry and Molecular Biosciences, The University of Queensland, St Lucia, QLD, 4072, Australia
**Email: stephen.sanderson@uq.edu.au*

Molecular dynamics (MD) simulations provide various methods for nanoscale flow modelling. Some are applicable to confined flows, while others model flow in the bulk. Although most methods appear conceptually simple, they are complicated by the need for a thermostat to prevent infinite heating. From this, a number of subtleties arise which may cause incorrect results, especially at high flow rates. This is particularly true when modelling bulk molecular flow, where all atom velocities include some streaming component which is not thermal (and should therefore not be thermostatted), and the streaming velocities are non-trivial due to rotational motion of molecules.

This talk gives an overview of key considerations when simulating flow, before focusing on the case of bulk molecular flow. As part of a Pawsey Centre for Extreme Scale Readiness (PaCER) project, we are extending the functionality of the popular MD package LAMMPS to allow for bulk molecular flow modelling using well-established, yet not widely implemented, algorithms which aim to avoid spurious effects at high flow rates. An outline is given of the applicability and key details of these algorithms, along with some preliminary results.

IL72 A new superstructure in beam sensitive cathode material revealed by multimodal stem combining ADF, IDPC and EDX mapping techniques

, Maria Meledina[1]*, Alexander Meledin[1], Ryan Shaw[1,]Eric G T Bosch[1], Ivan Lazić[1], Xiaochao Wu[2], Ulrich Simon[2], Boy Markus[1], Bert Freitag[1], Sorin Lazar[1], Paolo Longo[1]
[1]Thermo Fisher Scientific
[2]Institute of Inorganic Chemistry, RWTH Aachen University , Aachen , Germany
***Email:** *Maria.meledina@thermofisher.com*

In this work we exploited atomic resolution low dose techniques to investigate beam-sensitive cathode battery material. Cathode materials are obstinate candidates for TEM investigations due to their poor stability under the electron beam. Low electron dose should be applied in order to minimize radiolysis while imaging $LiCoPO_4$.

Here, we exploit simultaneous ADF-STEM and iDPC-STEM [2,3] imaging to investigate the $LiCoPO_4$ cathode material down to atomic scale, as iDPC-STEM allows for extremely low dose imaging of beam sensitive materials [4,5]. By combining the experimental and simulation results a superstructure at the surface of the $LiCoPO_4$ nanoparticle is revealed: every second Li site is partially occupied by higher Z-number atoms as periodic bright contrast is observed.

To confirm the proposed superstructure, EDX spectroscopy at atomic resolution is performed.

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IL73 Highly efficient wide band gap semiconductors for breakdown of perfluoroalkyl substances

Cameron J. Shearer,[1]* Rachael K. Matthews,[1] Mabel L. Day,[1] Mahmoud A. Hamza[1]

[1]*Department of Chemistry, The University of Adelaide, Adelaide, South Australia, Australia*
**Email: cameron.shearer@adelaide.edu.au*

Perovskite metal oxides, ABO_3 , are the current benchmark water-splitting photocatalysts with recent reports showing ~100% quantum efficiency ($SrTiO_3$ with 365 nm irradiation).[1-2] A major strategy to enhance photocatalytic performance is aliovalent doping.[3]

This presentation will investigate doping strategies of $ATaO_3$ (A = Li, K, Na) to enhance photocatalysis efficiency. Photocatalysts were prepared via high temperature solid state synthesis. The prepared photocatalysts were characterised with UV-Vis diffuse reflectance spectroscopy, XRD, SEM, Raman spectroscopy, and high-angle annular dark field (HAADF) STEM with energy-dispersive X-ray spectroscopy (EDS) and electron energy loss (EELS) mapping.

Photocatalytic performance was screened by monitoring the breakdown of an anionic organic test molecule (4-[(4-dimethylamino)phenylazo]benzenesulfonate) under irradiation from an LED array. Low levels of doping was able to significantly enhance the photocatalytic rate. The most active photocatalysts were then used for the degradation of perfluoroalkyl substances (PFAS). The wide bandgap semiconductors were found to have far greater efficiency for breaking the C-F bond, than TiO_2 benchmark photocatalyst.

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IL74 Harnessing motion via polymers: from ferroelectricity to electrostatics

Peter C. Sherrell,[1,2]*, Ronald T. Leon,[2] Andris Šutka,[3] Amanda V. Ellis[2]

[1] School of Science, RMIT University, Melbourne, Victoria 3001, Australia
[2] School of Chemical and Biomedical Engineering, University of Melbourne, Parkville, Victoria 3010, Australia
[3] Institute of Surface and Materials Engineering, Riga Technical University, Riga LV-1048, Latvia
**Email: peter.sherrell@rmit.edu.au*

Harvesting electrical energy from motion is a key challenge for powering small scale electronic devices, from the internet-of-things to implantable bionics. The two dominant mechanisms for converting motion to electricity within a material are the piezoelectric effect (deformation-to-electricity)[1] and the triboelectric (friction-to-electricity).[2] Polymers, as chemically stable and flexible materials, are ideal materials to exploit the piezoelectric and triboelectric effects for energy harvesting.

The triboelectric effect is often conflated with piezoelectricity, due to inconsistent testing methodologies,[3] and the very similar voltage and charge waveform outputs observed.[4] This is compounded by poor, often empirically derived, understanding of triboelectric charging between two materials. This talk will compare and contrast ferroelectric and electrostatic energy harvesting mechanisms, including approaches to isolate piezoelectric and triboelectric contributions by measurement techniques,[3] and signal analysis approaches.[4] These approaches will be complemented by developed mechanistic understanding linking materials chemistry,[5] and surface topography,[6] to predict triboelectric charging between two polymer materials. Finally, I will demonstrate that by combining these mechanistic understandings and analysis tools, polymer energy harvesting systems with dramatically enhanced mechanical-to-electrical conversion can be engineered.[7]

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IL75 Novel solvothermal synthetic designs for snse-based thermoelectric materials

Xiaolei Shi, Zhi-Gang Chen*

[1] School of Chemistry and Physics, Queensland University of Technology, Brisbane, QLD 4000, Australia
**Email: zhigang.chen@qut.edu.au*

SnSe has emerged as a promising thermoelectric material for practical applications due to its cost-effectiveness, low toxicity, and suitable bandgap. However, utilizing SnSe in thermoelectric devices presents challenges in simultaneously optimizing its thermoelectric and mechanical properties. This study provides a comprehensive summary of recent advancements in enhancing the thermoelectric and mechanical properties of bulk SnSe materials through solvothermal synthesis, drawing from our recent research. We discuss progress in synthesis techniques, characterization methods, enhancements in thermoelectric performance, and potential applications. Additionally, we address ongoing debates, strategies, and future prospects for the development of tin selenide-based thermoelectric materials and devices across diverse application scenarios.

IL76 Stretchable electronics based on single-walled carbon nanotubes

Chien-Chung Shih[1*]

[1]*Department of Chemical and Materials Engineering, National Yunlin University of Science and Technology*

**Email: shihcc@yuntech.edu.tw*

Single-walled carbon nanotubes (SWNTs) have been extensively researched for their potential in flexible and stretchable devices. SWNTs possess sevpieral attractive qualities, including high charge carrier mobility, mechanical flexibility, and compatibility with modern electronics. In this lecture, I will report our recent researches on SWNTs, covering three primary aspects: the purification process, the creation of stretchable and high -performance CNT transistors, and the design of stretchable micro-supercapacitors using SWNTs.

Industrial-scale production of SWNTs typically produce a mixture of ~2/3 semiconducting SWNTs (s-SWNTs) and 1/3 metallic SWNTs (m-SWNTs), as well as contaminants amorphous carbon and residual catalyst. Consequently, the purification of s-SWNTs is a critical step in the development of SWNT electronics. To tackle this challenge, a novel approach utilizing a semi-conjugated fluorene copolymer for precise SWNT sorting has been employed. This refined approach facilitates the polymer wrapping process within polar and bio-renewable solvents, culminating in commendable yields and unparalleled purity levels for s-SWNTs. In addition to purification procedures, we have successfully developed inherently stretchable transistors and integrated circuits using s-SWNTs on stretchable substrates. These transistors exhibit superior drive capabilities, rapid operational speeds, and broad integration possibilities. Furthermore, we have harnessed this technology to create stretchable SWNT-based micro-supercapacitors, addressing the critical requirement for efficient power sources. These advancements in device performance establish a robust technological foundation, significantly enhancing the capabilities of skin-like electronics and catalyzing a transformative revolution in related applications.

IL77 Soft Semiconductors for Stretchable Electronics, Light Harvesting and Sensing

Prashant Sonar [a, b,]

[a]*Professor and Former ARC Future Fellow, School of Chemistry and Physics, Centre of Material Science, Queensland University of Technology, Brisbane, Australia*
[b]*Centre for Biomedical Technology, Queensland University of Technology, Brisbane, *Email: sonar.prashant@qut.edu.au*

Next generation active electronic materials used in devices are undergoing continual improvements to generate devices that are high performance, lighter, flexible, stretchable, and more energy efficient with lower cost. Carbon based novel solution processable π-functional conjugated materials are the focus of intense academic and industrial research since they are important class of soft materials for large area electronics including transistors, displays, sensors and light harvesting devices. The active organic semiconducting materials are emerging due to their tunable light absorption/emission, interesting charge transport properties, relatively adequate HOMO-LUMO energies and ink formulation capability.

In my talk, I will explain the various classes of conjugated carbon-based soft semiconducting materials either as polymers, small molecules or quantum dots prepared via chemically and electrochemically using various novel aromatic conjugated building blocks.[1-22] In this presentation, the design, synthesis, optoelectronic properties, and device performance of novel advanced materials for field effect/electrochemical transistors, perovskite solar cells, light emitting diodes, optical sensors and various sensing devices will be discussed. Such materials and devices have great potential in future electronics, energy, health, and environmental monitoring.

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IL78 Engineering robust, fire-retardant advanced composites for electromagnetic interference shielding

Pingan Song,[1]*, Yongqian Shi [2]

[1] School of Agriculture and Environmental Science, University of Southern Queensland, Springfield 4300 Australia
[2] College of Environment and Safety Engineering, Fuzhou University, 2 Xueyuan Road, Fuzhou 350116, China.
**Email: pingan.song@usq.edu.au*

MXene aerogels have shown great potential for many important functional applications, in particular electromagnetic interference (EMI) shielding. However, it has been a grand challenge to create mechanically hyperelastic, air-stable, and durable MXene aerogels for enabling effective EMI protection at low concentrations due to the difficulties in achieving tailorable porous structures, excellent mechanical elasticity, and desired antioxidation capabilities of MXene in air. Here, we report a facile strategy for fabricating MXene composite aerogels by co-assembling MXene and cellulose nanofibers (CNFs) during freeze-drying followed by surface encapsulation with a fire-retardant thermoplastic polyurethane (TPU) elastomer. Because of the maximum utilization of pore structures of MXene, and conductive loss enhanced by multiple internal reflections, as-prepared composite aerogel with 3.14 wt.% of MXene exhibits an exceptionally high EMI shielding effectiveness of 93.5 dB, and an ultra-high MXene utilization efficiency of 2977.71 dB/g·g-1, tripling the values in previous works. Owing to multiple hydrogen bonding interactions and the TPU elastomer, the aerogel exhibits a hyperelastic feature with additional strength, excellent stability, and superior durability, as well as high fire safety. This work provides a facile strategy for creating multifunctional aerogels with great potential for applications in EMI protection, wearable devices, thermal management, pressure sensing, and intelligent fire-monitoring.

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IL79 An improved intermolecular interaction energy model for the prediction of free energies that determine crystal growth

Peter R. Spackman, [1]*, Julian D. Gale[1]

[1] *School of Molecular and Life Sciences, Curtin University,*
GPO Box U1987, Perth, WA 6845, Australia
**Email: peter.spackman@curtin.edu.au*

Accurate and fast models for intermolecular interactions provide quantitative insight into crystal packing, but their value can extend beyond neighbouring interactions into the prediction of lattice energies [1], and when combined with solvation models yield sensible estimates for solubilities for crystals in different solvents. We present both a new and improved CrystalExplorer interaction energy model [2,3], along with its application for predicting lattice energies, solubilities and the underlying thermodynamics guiding crystal growth from solution [4].

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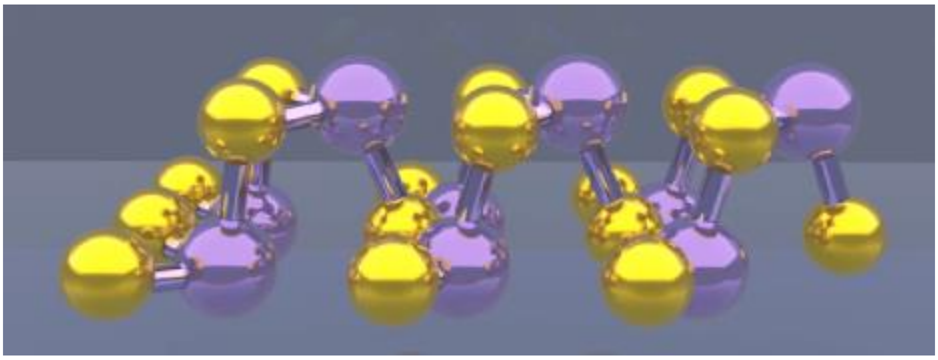
IL80 2D materials for flexible electronics and piezoelectric actuators

Michelle J.S. Spencer[1]*

[1]ARC Centre of Excellence in Future Low-Energy Electronics, School of Science, RMIT University, GPO Box 2476 Melbourne Victoria 3001 Australia
**Email: michelle.spencer@rmit.edu.com*

Wearable devices have increased in popularity with their ability to monitor one's health and track daily exercise. These devices still require batteries to power them and can be quite chunky. Two-dimensional (2D) materials have the ability to make the electronic component in these devices smaller, allowing for lighter, more flexible and smaller wearables to be developed. These materials can also be used as alternative power sources through conversion of mechanical energy into electrical energy and vice versa (i.e. piezoelectricity). The motion produced by such materials also has the potential to mimic the behavior of biological muscles for new applications, such as robotics or prosthetics. A number of 2D materials, such as MoS_2, have structures that make them flexible and highly piezoelectric, however, the responses achieved by these materials, and some others, is still not comparable to mammalian muscles. New materials with larger piezoelectric properties are needed. In this presentation I will discuss our work examining the electromechanical response of the 2D group IV monochalcogenides, SnS, SnSe, GeS and GeSe, using density functional theory (DFT) calculations [1]. We have demonstrated that upon electron and hole injection the monolayers expand and contract respectively, with SnS achieving piezoelectric responses greater than previously studied materials. We have also used DFT calculations to show how defects can be used to restore the piezoelectric properties of ultrathin sheets of ZnO [2].



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IL81 Precise defect engineering on graphitic carbon nitrides for boosted solar H_2 production

Dawei Su[a]

[a]*School of Mathematical and Physical Sciences, Faculty of Science, University of Technology Sydney, Broadway, NSW 2007, Australia.*

**Email: dawei.su@uts.edu.au*

Abstract: Defect engineering has been regarded as an "all-in-one strategy" to alleviate the insufficient solar utilization in g-C_3N_4. However, without appropriate modification, the defect benefits would be partly offset due to the formation of deep localized defect states and deteriorated surface states, lowering the photocarrier separation efficiency. To this end, we discreetly designed the defective g-C_3N_4 with both S dopants and N vacancies via a dual-solvent-assisted synthetic approach. The precise defect control was realized by the addition of ethylene glycol into precursor formation and molten sulfur into the pyrolysis process, which simultaneously induced DCN-ES with shallow defect states. These shallow defect energy levels could act as a temporary electron reservoir, which is critical to evoke the migrated electrons from CB with moderate trapping ability, thus suppressing the bulky photocarrier recombination. Additionally, the optimized surface states of DCN-ES were also demonstrated by the highest electron-trapping resistance ($R_{trapping}$) of 9.56×10^3 Ω cm^2 and the slowest decay kinetics of surface carriers (0.057 s^{-1}), which guaranteed the smooth surface charge transfer rather than being the recombination sites. As a result, DCN-ES exhibited a superior H_2 evolution rate of 4219.9 μmol g^{-1} h^{-1}, which is 29.1-fold higher than unmodified g-C_3N_4.[1]

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IL82 Enhanced interactions of interlayer excitons in free-standing heterobilayers

Xueqian Sun[1], Yi Zhu[1], Hao Qin[1], Boqing Liu[1], Yilin Tang[1], Tieyu Lü[2], Sharidya Rahman[1], Tanju Yildirim[3], and Yuerui Lu[1,4*]

[1]*School of Engineering, College of Engineering and Computer Science, the Australian National University, Canberra, ACT, 2601, Australia*
[2]*Department of Physics and Institute of Theoretical Physics and Astrophysics, Xiamen University, Xiamen, 361005, China*
[3]*Center for Functional Sensor & Actuator (CFSN), National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0044, Japan*
[4]*Australian Research Council Centre of Excellence for Quantum Computation and Communication Technology, the Australian National University, Canberra, ACT, 2601 Australia*
**Email: u5134679@anu.edu.au*

Strong, long-range dipole–dipole interactions between interlayer excitons (IXs) can lead to new multiparticle correlation regimes, which drive the system into distinct quantum and classical phases, including dipolar liquids, crystals and superfluids. Both repulsive and attractive dipole–dipole interactions have been theoretically predicted between IXs in a semiconductor bilayer, but only repulsive interactions have been reported experimentally so far. This study investigated free-standing, twisted (51°, 53°, 45°) tungsten diselenide/tungsten disulfide (WSe_2/WS_2) heterobilayers, in which we observed a transition in the nature of dipolar interactions among IXs, from repulsive to attractive. This was caused by quantum-exchange-correlation effects, leading to the appearance of a robust interlayer biexciton phase (formed by two IXs), which has been theoretically predicted but never observed before in experiments. The reduced dielectric screening in a free-standing heterobilayer not only resulted in a much higher formation efficiency of IXs, but also led to strongly enhanced dipole–dipole interactions, which enabled us to observe the many-body correlations of pristine IXs at the two-dimensional quantum limit. In addition, we firstly observed several emission peaks from moiré-trapped IXs at room temperature in a well-aligned, free-standing WSe_2/WS_2 heterobilayer. Our findings open avenues for exploring new quantum phases with potential for applications in non-linear optics.

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IL83 Materials design for renewable energy storage systems

Bing Sun [1]*

[1] *Centre for Clean Energy Technology, School of Mathematical and Physical Sciences, Faculty of Science, University of Technology Sydney, Ultimo, NSW 2007, Australia.*

**Email: bing.sun@uts.edu.au*

Owing to the superior high energy density, metal air batteries (e.g. lithium–oxygen batteries and sodium–oxygen batteries) have been considered promising advanced battery systems to meet today's stringent requirements as the power source for electric vehicles (EVs) and renewable energy storage. However, the development of metal air batteries is still constrained by several serious challenges, including uncontrolled side reactions, low energy efficiency and poor cycling life. The electrochemical performances of lithium–oxygen batteries await dramatic improvement in the design of porous oxygen cathodes, efficient electrocatalysts and stable metal anodes.

Herein, we present the research outcomes from our group on materials innovation for rechargeable metal air batteries. First, the family of metal air batteries will be introduced. Second, the design of porous carbon-based materials and redox mediators for high-performance air (oxygen) cathodes will be discussed. Third, facile and effective methods to enhance the electrochemical performance of lithium/sodium metal anodes will be presented, including electrolyte optimization, three-dimensional current collector design, and dual interface engineering on lithium/sodium metal anodes.

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IL84 Correlation of charge carrier dynamics with the performance of metal halide perovskite solar cells

Wakana Matsuda,[1,2] Keishiro Goshima,[3,4] Yasuhiro Tachibana[1,3,*]

[1] Forefront Research Center, Graduate School of Science, Osaka University, Toyonaka, Osaka, 560-0043, Japan
[2] Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Katsura, Kyoto 615-8510, Japan
[3] School of Engineering, RMIT University, Bundoora, Victoria 3083, Australia
[4] Aichi Institute of Technology, 1247, Yachigusa, Yakusa, Toyota, Aichi, Japan
**Email: yasuhiro.tachibana@rmit.edu.au; tachibana.yasuhiro.sci@osaka-u.ac.jp*

Perovskite solar cells have been recognized as a newly emerging solar cell with the potential of achieving high efficiency with a low cost fabrication process. In particular, facile solution processed cell fabrication facilitated rapid development of optimum cell structure and composition. Over the last few years, the cell efficiency has reached 26%.

High charge separation efficiency and swift charge transport with minimum charge recombination are required to improve solar cell performance. Intensive studies have focused on monitoring charge dissociation, charge transport and interfacial charge transfer dynamics including interfacial charge recombination in perovskite solar cells.[1-5] Several parameters have been identified to influence these charge carrier dynamics, and therefore solar cell performance.[1-5] Clarifying these parameters is extremely important to understand the charge transfer mechanisms to further improve solar cell performance.

In this presentation, we will present parameters controlling charge separation and recombination dynamics at the perovskite interfaces employing a series of transient absorption and emission spectroscopies. Correlation of the key parameters with the solar cell performance will be discussed [1-5].

This work was partly supported by JSPS KAKENHI Grant (19H02813) and (22H02182), and the Collaborative Research Program of Institute for Chemical Research, Kyoto University (grant number 2023-45 and 2022-99), Japan. We would like to acknowledge supports from the Australia-Japan Foundation for the international collaborative project. We also acknowledge supports from ARC LIEF fund (LE200100051 and LE170100235), Australia and School of Engineering in RMIT University, and Forefront Research Center, Faculty of Science at Osaka University.

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IL85 Multifunctional materials with aggregation-induced emission features

Youhong Tang *

Institute for NanoScale Science and Technology, Medical Device Research Institute, College of Science and Technology, Flinders University, South Australia 5042, Australia
**Email: youhong.tang@flinders.edu.au*

Aggregation-induced emission (AIE) is a unique and abnormal fluorescence phenomenon that has attracted increasing research interest over the past decades. Since its discovery in 2001, many AIE-active molecules with different structure, functional groups and optical properties have been reported. These AIE-active molecules can be further utilized to fabricate various functional materials, which have exhibited great potential for different applications [1]. The multifunctional materials with AIEgen inside created a unique research direction in both functional materials and AIE research communities. In this talk, the progress of combining polymers with AIEgens to form multifunctional materials has been updated, especially their applications for visualization, monitoring, sensing, and detecting have been emphasized. A few case studies in our group for AIE hydrogels in biomedical applications have been highlighted [2-4].

This significant strategy in multi-functionalized materials with AIE features has the potential for developing more efficient techniques for characterizing advanced nanomaterials and understanding biological processes and detection methodologies [5].

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IL86 Cobalt-catalyzed biomass conversion to functional carbon-based catalysts for environmental catalysis

Wenjie Tian[1]*

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

**Email: wenjie.tian@adelaide.edu.au*

Advanced oxidation processes utilizing peroxymonosulfate (PMS) activation are emerging as promising solutions for removing persistent organic pollutants in water[1]. Carbon-based catalysts derived from abundant and low-cost biomass are sustainable and promising for PMS activation. Pristine carbons usually have low or modest catalytic activity, and modifying them with transition metals, is an effective way to introduce more favorable active sites. The study investigates four typical cobalt salts for pyrolytic biomass conversion, finding that the melting point of cobalt salts is crucial for carbon structure formation[2]. Cobalt salts with low melting points could be trapped in a biomass flower precursor, promoting mesopore formation and catalyzing the graphitization process, forming mesoporous carbon matrixes with Co@graphitic-C nanoparticles and trace isolated Co atoms. By contrast, $CoSO_4$, with a high melting point, produces an amorphous carbon/Co9S8 nanoparticle composite. $Co@C\text{-}NO_3$ and $Co_9S_8@C\text{-}SO_4$ demonstrated the best performance in PMS activation for bisphenol A degradation, with distinct catalytic mechanisms due to different types of active sites. $Co@C\text{-}NO_3$/PMS shows multiple nonradical/radical pathways, while Co_9S_8@C-SO4/PMS demonstrates a selective sulfate radical-based reaction pathway. The catalysts showed excellent multiple organic pollutant removal performance in real water and good regeneration properties. This study offers novel insights into the rational design of biomass-derived carbon-based catalysts with desired active sites to meet different catalytic demands. This research contributes to the field by providing insights into the rational design of biomass-derived carbon-based catalysts, which can be tailored to meet different catalytic demands, and by demonstrating the efficacy of these catalysts in real water conditions.

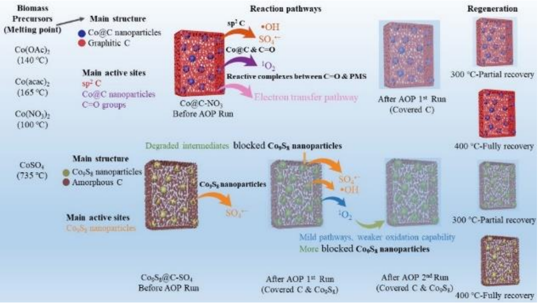

Figure 1 The influences of cobalt precursors on the structures of biomass-derived carbons and their performance in PMS activation.

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IL87 Decorated metal branched nanoparticle catalysts

Richard D Tilley[1]*

[1] School of Chemistry and Electron Microscope Unit, UNSW
**Email:* r.tilley@unsw.edu.au*

The primary challenge for high-performance nanoparticle catalysts is the atomic-level control of active sites. In this talk the evolution of state-of-the-art synthesis of metal nanoparticle catalysis with atomic-level control will be discussed. A range of concepts will be discussed including (i) using nanoparticles with specific shapes to expose specific facets to enhance catalytic stability for oxygen evolution, (ii) how these nanoparticles can be decorated with a second metal to form islands that have strain for enhanced activity for hydrogen evolution and (iii) how island can be spread to form single atom catalysts resilient to CO poisoning for methanol oxidation. Developments in the transmission electron microscopy (TEM) atomic scale characterization of active sites will also be illustrated with the discussion of different imaging modes and how *in situ* TEM can be used to elucidate synthetic reaction mechanisms (Fig 1).

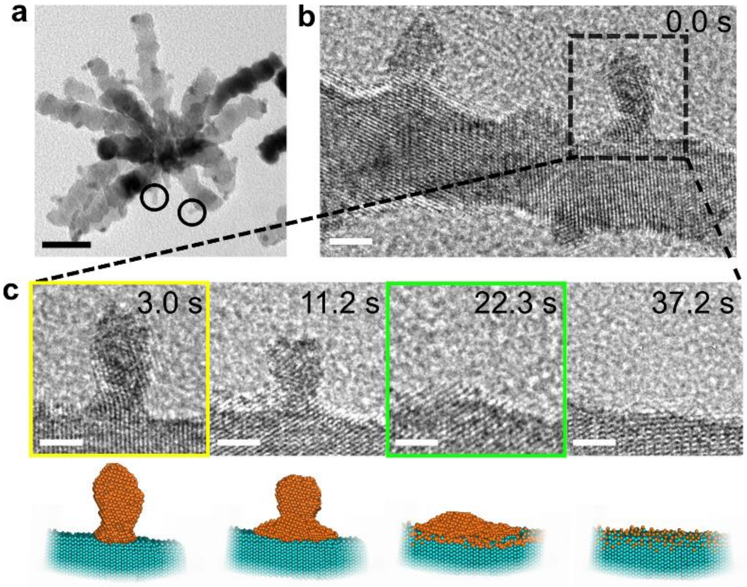

Figure 1. In situ TEM of the spreading process of Pt islands on a Ru branched nanoparticle to form CO resistant single atom catalysts.

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IL88 Graphitic nanoflakes modulate amyloid fibril formation: effects of size and oxidation

Alexa Kamboukos[1], Billy Williams-Noonan,[2] Patrick Charchar,[1] Irene Yarovsky,[1] Nevena Todorova[1*]

[1] School of Engineering, RMIT University, Melbourne, Australia
[2] School of Science, RMIT University, Melbourne, Australia
**Email: nevena.todorova@rmit.edu.au*

Amyloid fibril formation is complex process characterised by the misfolding and aggregation of proteins into highly order fibrillar structures. The deposition and accumulation of these fibrillar deposits in human tissues have been linked to a variety of debilitating diseases [1]. Human amylin, an inherently disordered protein, undergoes abnormal unfolding and aggregation, which is linked to the onset of type-II diabetes. Graphitic nanomaterials have shown promise in mitigating amyloid diseases, but their optimal design remains uncertain [2]. In this study, we employed enhanced sampling molecular dynamics simulations [3] to conduct a comprehensive analysis of the structural and adsorption characteristics of amylin onto nine distinct graphitic nanoflakes. These nanoflakes exhibited variations in dimensions and surface functionalisation, factors that were previously demonstrated to influence their curvature, roughness, and hydration properties within biological environments [4]. Our research reveals a close intrinsic relationship between protein adsorption and both the size of the graphitic surface and the extent of surface oxidation. Notably, our findings indicate that by tailoring the oxygen concentration and surface patterning of graphene oxide (GO), it is possible to control the binding preferences and induce conformational changes in amylin. This, in turn, influences the likelihood of fibril formation. The atomistic insights from this study offer valuable guidance for the development of graphitic nanoflakes that can effectively regulate protein aggregation. These findings hold promise for advancing our understanding of amyloid diseases and developing targeted therapeutic interventions.

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IL89 Engineering scalable electrocatalysts for renewable hydrogen production at a global scale

Antonio Tricoli

[1] Nanotechnology Research Laboratory, Faculty of Engineering, University of Sydney
[2] Nanotechnology Research Laboratory, Research School of Chemistry, Australian National University
**Email: antonio.tricoli@sydney.edu.au*

Protecting our environment while sustaining industrial and economic growth is an ambitious and essential aim that needs to be achieved at a global scale to be successful. Governments have expressed worldwide support to commit to net-zero emission targets to mitigate climate change. This requires development of new technologies to rapidly decrease our reliance on fossil-fuel resources. Chemical storage of renewable energy harvested from solar farms and wind by electrochemical hydrogen production is an attractive approach to enable the export of renewable energy to countries with less access to renewable energy sources and/or very high population density. Electrochemical hydrogen production is also beneficial as an intermediary large scale energy storage approach for stabilization of the electrical grid and on-demand off-the-grid power generation. While a variety of carbon-emission-free electrochemical hydrogen production technologies have reached commercial maturity, they still rely on rare and expensive electrocatalyst that undermines their inherent scalability below that required for adoption of hydrogen as global energy carrier. Furthermore, the high cost and poor lifetime of these rare catalysts increase the cost electrochemical production of hydrogen hindering its economic sustainability.

In this paper, we will discuss emerging approaches for the use of low-cost earth abundant materials as efficient electrocatalysts for green hydrogen and e-fuels production [1]. The multi-scale engineering of nano-micro materials and their integration in effective macro- scale morphologies will be presented as successful strategy for the use of a variety of earth-abundant rock forming elements as electrodes and membranes of electrolysers. The need to overcome the limitations imposed by single constituent such as the poor electrical conductivity of iron oxide and/or surface activity of manganese oxide will be demonstrated by the fabrication of highly performing nano-micro composite electrocatalysts made of carefully controlled hierarchical structures. We will showcase the use of the latest generation of flame-aerosol synthesis reactors for the direct roll-to-roll fabrication of electrodes for alkaline and acidic electrolysers, demonstrating a scalable path for the low-cost production of green hydrogen from renewable energy sources. The advantages and challenges of the flame synthesis route will be critically discussed providing directions for its optimization as a scalable technology for electrocatalyst production.

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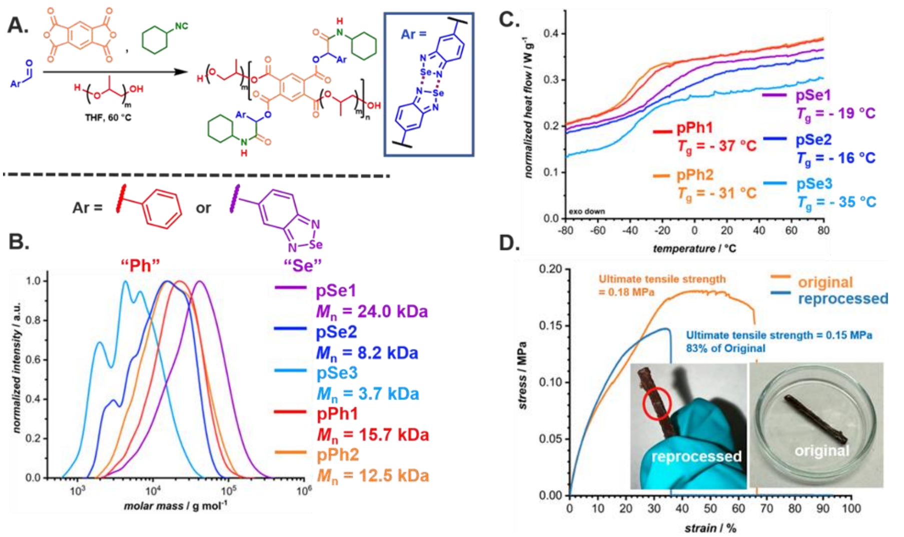
IL90 Dynamic chalcogen squares for material and topological control over macromolecules

Aaron H. Bui,[1] Anne Fernando Pulle,[1] Aaron S. Micallef,[1,2] Jacob J. Lessard,[3] Bryan T. Tuten[1]*

[1] School of Chemistry and Physics, Centre for Materials Science, Queensland University of Technology, 2 George Street, Brisbane, QLD, 4000, Australia
[2] Central Analytical Research Facility, Queensland University of Technology, 2 George Street, Brisbane, QLD, Australia
[3] Beckman Institute for Advanced Science and Technology and Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, United States
**Email: bryan.tuten@qut.edu.au*



Overview of selenadiazoles as dynamic material motifs. A) Synthesis of selenadiazole-containing polymer via tandem Passerini polymerization. B) Various molecular weights of selenadiazole-containing and control polymers. C) Controlling glass transition temperature of soft matter materials via incorporation of chalcogen squares. D)Self-healing soft matter materials via dynamic non-covalent chalcogen bonding.

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.

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IL91 Development of robust flexible quasi-solid-state ag-zn batteries with long cycle life

Tao Wan[1]*, Yanzhe Zhu, Dewei Chu

[1] School of Materials Science and Engineering,
University of New South Wales, Sydney 2052, Australia
**Email: tao.wan@unsw.edu.au*

Traditional Ag-Zn batteries have been commercialized in various small electronics, but the batteries suffer from inferior cycling performance, low areal capacity, and poor mechanical flexibility, hindering their practical application in next generation electronics. In this work, flexible quasi-solid-state Ag-Zn batteries with high areal capacity and long cycle stability are developed by using mild electrolyte and binder-free electrodes. The electrochemical performance of the batteries has been significantly enhanced through engineering the electrodes and electrolyte. 3D copper foam is used as current collector to impede the growth of Zn dendrite for high cycle stability, and the cathode with a core-shell structure is developed to improve the areal capacity and alleviate undesired Ag migration. The resulting batteries with dendrite-free anode and stable cathode demonstrate a remarkable capacity retention at high current density. The developed high-performance flexible Ag-Zn batteries can operate in extreme conditions, such as being bent, twisted, cut, put on fire, and sealed in solid ice, and they can power various electronics for practical applications, such as electronic ink display, temperature and humidity sensor, motion sensor, and heart rate sensor. This work provides guidelines to design electrodes and electrolyte towards high-performance flexible Ag-Zn batteries.

IL92 Affordable double-reference approach for simulating electrified solid/water interfaces

Jack Hinsch,[1] Assil Bouzid,[2] Yun Wang[1]*

[1] Centre for Catalysis and Clean Energy, School of Environment and Science, Griffith University, Gold Coast, QLD 4222, Australia
[2] Institut de Recherche sur les Céramiques (IRCER), UMR CNRS 7315-Université de Limoges, Limoges 87068, France
**Email: yun.wang@griffith.edu.au*

Recently, we developed an innovative and cost-effective approach based on the Grand Canonical Density Functional Theory (GC-DFT) method to investigate the behaviour and properties of the electrified solid-water system [1]. We used a hybrid approach with a "sandwich" design to combine explicit and implicit solvation methods, which can overcome convergence issues and provide more reliable results. Our research demonstrates that while the implicit solvation model can reduce computational costs, the hybrid approach better considers the interactions of water molecules, which are crucial for describing the electric double layer.

Furthermore, our analysis of the structural properties of the interface emphasizes the significant role played by the orientation and position of water molecules in determining the system's PZC (potential of zero charge) and double-layer capacitance. Additionally, the relationship between electrochemical properties, including double-layer charge and capacitance and the applied bias potential derived from our GC-DFT results show a correlation with two distinct linear domains at the electrified Pt(111)/water interface, in good agreement with experimental measurements. We also observed variations in the adsorption energies of hydrogen on Pt at different potentials, indicating the impact of hydrogen adsorption on the system's performance.

Our developed affordable GC-DFT approach provides researchers with a valuable and efficient means to enhance their understanding of electrified solid-liquid interfaces. By combining the advantages of both implicit and explicit solvation methods, our approach offers an accurate description of the interactions and properties of these interfaces while minimizing computational costs. The effectiveness of our approach is further validated by the agreement between our findings and those reported in experiments and expensive AIMD (ab initio molecular dynamics) simulations.

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IL93 Advanced chemical sensing enabled by low-dimensional nanomaterials

Yichao Wang [1*]

[1] *School of Engineering, Design and Built Environment, Western Sydney University*
**Email: yichao.wang@westernsydney.edu.au*

The incorporation of low-dimensional (LD) nanomaterials into the realm of chemical sensing technologies has emerged as a pioneering and promising strategy, offering the potential for remarkable progress in sensitivities, selectivity and adaptability [1,2]. LD-nanomaterials, in contract to their bulk counterparts, exhibit several unique properties that make them highly attractive for chemical sensing applications [3,4]. These properties include large surface area, unique electronic and optical characteristics, tunable energy band diagrams and intercalatable morphologies that can be fine-tuned when exposed to external chemical molecules. These inherent characteristics establish LD-nanomaterials as an ideal platform for chemical sensing applications, enabling the detection of a wide range of chemical molecules.

In this presentation, I will share our research progress in the development of low-dimensional transition metal dichalcogenides and oxides and their applications in detecting ions, biomolecules and gas molecules, showing their potential to address critical challenges in the fields such as environmental monitoring and healthcare. The sensors enabled by LD-nanomaterials are very sensitive to the external stimuli from the target molecules. Through manipulation of the electrochemical and optical responses, the sensitivity, selectivity and detection limits in these sensors are optimized.

Additionally, I will discuss our recent research effort in plant nanobionic sensors and their uses for real-time detection and monitoring of plant stress-induced signaling molecules. This timely and non-invasive approach holds great promise for advancing our understanding of plant physiology and aiding in the development of strategies for improved crop management and sustainability.

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IL94 2D bismuth-based nanomaterials for catalytic applications

Dr Liang Wang [1]*

[1]*The Centre for Catalysis and Clean Energy, Griffith University, Gold Coast Campus, QLD, 4222 Australia*
**Email: liang.wang@griffith.edu.au*

Owing to unique structures and properties, 2D layered materials have exhibited great potentials for catalysis for clean energy and environmental sustainability.[1] Among these, 2D Bi-based layered materials possessing intriguing characteristics have attracted tremendous attention.[2] However, practical applications of these Bi-based semiconductors in catalysis remain a challenge due to their low catalytic efficiency. In most cases of them, the large band gap and unsuitable band-energy positions in band structures can lead to limited visible-light absorption and low solar-conversion efficiency.[3] Additionally, the low concentration of active sites on the exposed accessible surfaces is also a key factor limiting their catalytic efficiencies.[4] In this talk, I will present my recent research progresses on developing structural engineering strategies to overcome these limitations, including constituent adjustment, vacancy engineering, and construction of 2D hetero-structures.[5-7]

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IL95 Curvature-dependent performance of oxidized carbon nanotubes for hydrogen peroxide synthesis

Li WEI, [1*]

[1] *School of Chemical and Biomolecular Engineering, The University of Sydney, Darlington, NSW, AU, 2006*

**Email: l.wei@sydney.edyu.au*

Surface oxidized carbon nanotube (o-CNTs) can produce sustainable hydrogen peroxide (H_2O_2) by two-electron transferred oxygen reduction reaction (2e-ORR). The C atoms neighboring to surface epoxy (C-O-C) groups are recognized as active sites. Herein, we report the CNT curvature, or diameter, dependent ORR activity of o-CNT catalysts. Computation modelling suggests that the curvature can alter epoxy group geometry, exerting greater strain on the C-O bond in smaller diameter o-CNTs that leads to improved activity. This theoretical prediction is further experimentally validated by five o-CNTs of different diameters but comparable oxygenous groups. The o-CNT with the smallest diameter (8 nm) delivers the highest H_2O_2 Faradaic efficiency (>85%, or molar selectivity >90%) and an impressive mass activity of 161 A g^{-1} at 0.65 V, as one of the best carbon-based catalysts reported recently. This curvature effect provides a new strategy to design and synthesize efficient electrocatalysts for peroxide production and beyond.

Email abstracts as an attachment to materials.div@raci.org.au before the abstract deadline midnight **Sunday 24 September 2023.**

IL96 Controlling halide segregation in mixed-halide perovskites

Asaph Widmer-Cooper, [1]*

[1] Australian Research Council Centre of Excellence in Exciton Science, School of Chemistry,
University of Sydney, Sydney, NSW 2006, Australia.
**Email: asaph.widmer-cooper@sydney.edu.au*

Metal halide perovskites (MHPs) are a promising class of materials for optoelectronic applications that are energy efficient, printable, low-cost and solution processable.[1] A key requirement for many MHP applications, including tandem solar cells, LEDs, photodetectors and lasers, is the ability to tune the material bandgap by varying the halide composition, i.e. the ratio of I^-, Br^- and Cl^-. This can be well controlled at the manufacturing stage by changing the relative amounts of halide precursors in solution. However, in practice, the performance of devices made using mixed-halide perovskites has been limited by poor material stability as the halides phase segregate upon light exposure. This leads to localized changes in the material bandgap which in turn affect the optoelectronic properties. This effect is known as photoinduced halide-ion segregation (PHS). Understanding its origin and how to reverse it, is therefore vital to develop stable MHP devices and to promote their adoption into the market.

I this talk, I will discuss a model that we have developed for explaining the complex effects of light and heat on PHS, including the ability to reverse segregation at higher light intensity.[2] Our model is based on the Ising spin theory and on the hypothesis of polaron mediated segregation. In the model, halide ions are represented as nodes on a lattice that can exchange position with neighboring ions. The exchange depends on the interaction felt with neighbors and with polarons. Simulations of photoinduced halide migration within single crystals have been performed using a Monte Carlo (MC) algorithm which, akin to Kinetic MC, allows the simulation to resemble the time evolution of an actual phase space trajectory as the system approaches equilibrium. These simulations show excellent agreement with experimental results and help settle the ongoing debate about what mechanism is ultimately responsible for PHS, with potential new applications for MHPs.

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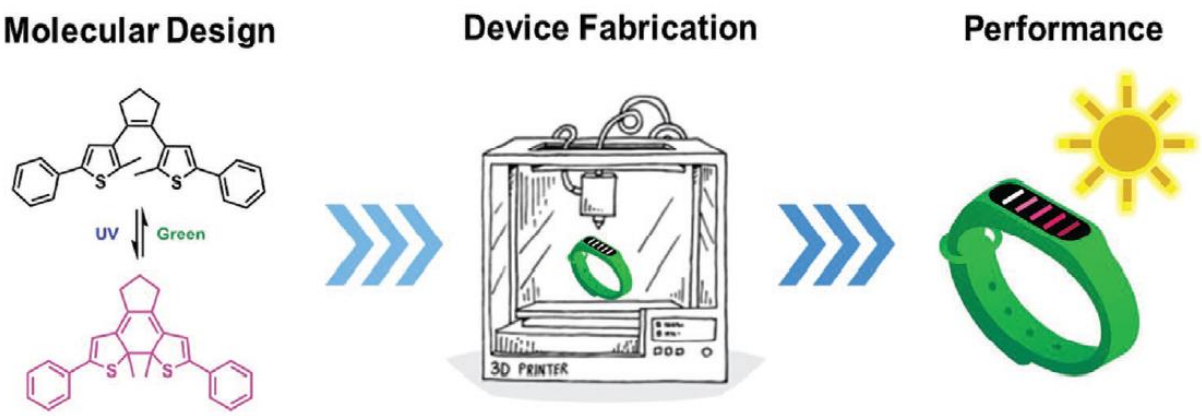
IL97 Shining bright: diarylethene photoswitches illuminate wearable uv sensors

Sandra Wiedbrauk,[1,2] Lauren E. Blackwell,[1] Heather McKinnon,[3] Levi Swann,[3] Nathan R. B. Boase[1,2]*

[1] Centre for Materials Science, Queensland University of Technology, Brisbane
[2] School of Chemistry and Physics, Queensland University of Technology, Brisbane
[3] School of Design, Queensland University of Technology, Brisbane

**Email: Sandra.wiedbrauk@qut.edu.au*

Approximately two out of three Australians will be diagnosed with skin cancer before reaching the age of 70. Despite ongoing educational campaigns, the incidence of skin cancer continues to rise, despite being a preventable form of cancer primarily caused by overexposure to UV light. We introduce a novel renewable UV sensor designed to raise awareness of UV overexposure.[1] These sensors employ diarylethene photoswitches that undergo a darkening process when exposed to sunlight and can be efficiently reset to a colorless state with green light in a short period of time. This color-changing property provides a straightforward method for monitoring UV exposure, offering visual feedback to users. Moreover, additional chromophores can fine-tune the UV sensitivity of these devices to cater to various skin types. These photoswitches have been incorporated into a variety of materials, enabling the 3D lithographic printing of customizable consumer products. Through collaboration with the School of Design, we have developed fashionable wearable sensors designed to encourage individuals to seamlessly integrate them into their daily routines.



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IL98 Stable perovskite quantum dots light-emitting diodes with high efficiency

Chaoyu Xiang[1]*, Xuanyu Zhang[1,2]

[1] First Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Science, Ningbo, Zhejiang, 315201, China
[2] Nottingham Ningbo China Beacons of Excellence Research and Innovation Institute, Ningbo 315040, China
**Email: xiangchaoyu@nimte.ac.cn*

Perovskite nanocrystals for light-emitting diodes were often synthesized by uncontrollable metathesis reactions, suffering from low product yield, nonuniform growth, and poor stability. Herein, by controlling the nucleation kinetics with high dissociation constant (Ka or Kb) acids or bases, homogenous one-route nucleation of perovskite nanocrystals was achieved as the cluster intermediates were eliminated. The stable, shape uniform, and narrow size distribution green nanocrystals were synthesized. The perovskite nanocrystal film exhibited excellent stability in 80% humidity air with only a 10% photoluminescence intensity drop after 16 hours. Efficient and stable electroluminescence was demonstrated with an FWHM of 16 nm at 517 nm. The green devices showed a peak EQE of 24.13% with a lifetime T_{50} of 54 min at 10000 cd/m^2. The performance is the highest among the perovskite QLEDs.

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IL99 Interfacial solar evaporation for environmental applications

Haolan Xu[1]*

[1]*Future Industries Institute, University of South Australia, Mawson Lakes Campus, Adelaide, Australia, SA 5095*
**Email: haolan.xu@unisa.edu.au*

Interfacial solar evaporation (ISE) is a promising technology to utilize solar light as the sole energy source for accelerated water evaporation [1]. It has been mainly utilized for seawater desalination and industry wastewater treatment [2]. During the last several years, great effort has been devoted to developing efficient photothermal materials and evaporators to improve energy efficiency and evaporation rate [3,5]. Based on this, new applications of ISE have also been explored. In this presentation, we will introduce the promising applications of ISE in contaminated soil and saline soil remediation, as well as floating solar sea farm for food and clean water production [6-8].

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IL100 Development of complex oxide materials for CO_2 electrolysis

Xiaomin Xu[1]*, Zongping Shao[1]*

[1] *WA School of Mines: Minerals, Energy and Chemical Engineering (WASM-MECE), Curtin University, Perth, WA, 6102 Australia*
**Email: xiaomin.xu@curtin.edu.au, zongping.shao@curtin.edu.au*

CO_2 electrolysis powered by renewables-generated electricity represents one promising approach to reducing carbon emissions while producing high value fuels or chemicals. This technology, however, is largely impeded by a lack of efficient catalysts toward the anodic oxygen evolution reaction (OER)[1-5] and cathodic CO_2 reduction reaction (CO_2RR).[6-10] Complex oxides are a group of materials that feature flexibility in composition and structure, thus offering tunability in electrocatalytic properties. Here, we summarise our recent findings in the development of non-precious metal-based perovskite-type oxides for catalysing the OER. We highlight how various materials engineering approaches including doping, introducing cation deficiency, and forming composites can lead to enhanced OER catalysis following an emerging lattice-oxygen mediated reaction path. We also identify a Cu-based complex oxide with constituting elements of yttrium and barium for highly active and selective CO_2RR showing enhanced formation of multicarbon products (C_{2+}). We report that the oxygen vacancy of this complex oxide can be leveraged to control the oxidation state of Cu, which is further correlated with the C_{2+} selectivity. The optimised catalyst achieves high C_{2+} selectivity of 60-70% at a potential of -0.8 to -1.2 V versus the reversible hydrogen electrode, comparing favourably to that of oxide-derived Cu catalysts. We expect that these findings can have implications for the development of improved catalysts for advancing the CO_2 electrolysis technology.

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IL101 Towards reliable quality control and standardization of graphene related 2d materials (GR2Ms) by thermogravimetric analysis (TGA)

Pei Lay Yap,[1,2]*, Dusan Losic[1,2]

[1] *School of Chemical Engineering, ARC Hub for Graphene Enabled Industry Transformation,* [2] *ARC Research Hub for Advanced Manufacturing with 2D Materials,*
The University of Adelaide, Adelaide, SA
5005, Australia
**Email: peilay.yap@adelaide.edu.au*

Counterfeits in the supply chain of emerging graphene and its derivatives have become a concerning issue that brings negative impact on this growing industry.[1] The absence of rapid, reliable and low cost standardization method for quality control of industrially manufactured graphene materials is a pressing problem.[2] The common and recommended methods for the characterization of graphene materials including transmission electron microscopy (TEM), atomic force microscopy (AFM), and Raman spectroscopy based on spot analysis are limited by their localized technique that failed to provide the properties of “bulk” graphene powder at a large scale.[3] Moreover, these techniques require skilled technical operators, time-consuming, and high cost. To address these challenges, TGA is developed and demonstrated as a rapid, reliable and low-cost characterization technique for quality control and standardization of GR2Ms to facilitate their lab to industrial translation. The performance of the developed TGA method was evaluated by a series of selected parameters including the number of mass loss steps, thermal stability, temperature of maximum mass change rate (T_{max}) for each decomposition step, and composition. The application of the developed TGA technique for chemical characterization of GR2Ms was successfully validated by an interlaboratory comparison (ILC) study using three typical types of GR2Ms powder with the involvement of 12 international laboratories across 5 continents and different organizations.[3] The outcomes of this ILC study with recommended improvement of TGA method will be implemented in a new standard for characterization of GR2Ms (*ISO/IEC standard “NWI 23359 Nanotechnologies Chemical characterization of graphene-related two-dimensional materials from powders and dispersions*”.[3]

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IL102 Development of high magnetization materials by nanoengineering

Jiabao Yi[1]*
**Email* jiabao.yi@newcastle.edu.au

[1]*Global Innovative Center for Advanced Nanomaterials, School of Engineering, University of Newcastle,Callaghan, 2308*

High magnetization materials are strongly required for the fabrication of advanced multifunctional magnetic materials and devices, whereas, the development of high magnetization materials is extremely slow. In this talk, I will propose a new strategy to achieve high magnetization above room temperature by nanoengineering. In the study of oxide based diluted magnetic semiconductors, metallic clusters have shown enhanced magnetization 【1,2】. We control the deposition parameters for 5% Co-TiO_2 to form effective subsitional doping or clusters 【3,4】. The substitional doping results in relatively low magnetic moment of Co. However, an enhanced magnetic moment up to 3.5 μ_B has been oberved in Co clusters, which is confirmed by X-ray magnetic circular dichroism (XMCD) and first principle calculations. The work suggests confinement effect can induce high magnetization. In another work, we utlize confinement effect to fabricate Ni/NiO nanocomposite to achieve a magnetization as high as 660 emu/cm^3, compared that of pure Ni (480 emu/cm^3) at room temperature【5】, suggesting that nanoclusters of antiferromagnetic oxide can be utilized for the fabrication of high magnetization materials. This project has provided a new technique to achieve high magnetization materials.

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IL103 Enhanced gating effects in responsive sub-nanofluidic ion channels

Huacheng Zhang [1]*

[1] *Chemical and Environmental Engineering, School of Engineering, RMIT University,*
Melbourne, Victoria 3000, Australia
**Email: huacheng.zhang@rmit.edu.au*

The smart regulation of ion flow in biological ion channels (BICs) is vital to life. In general, intelligent BICs possess three main functions: (i) to selectively transfer specific ions, (ii) to quickly conduct specific ions, and (iii) to responsively control the flow of ions. Since the early exploration of potassium (K^+) and sodium (Na^+) channels began in the 1950s, the gating behaviors of BICs have been investigated for more than 70 years. Taking the first reported voltage-gated ion transport process as an example, a gate, which acts as the voltage sensor in BICs, detects variation in the membrane voltage, triggering the opening and closing of the ion channels. BICs usually have strong gating effects with an extraordinarily high gating ratio, which can be up to infinity for channels with zero-current closed states. Inspired by nature, artificial ion channels (AICs) have been constructed to control ion permeation intelligently. Since 2004, a wide range of AICs have been developed to regulate the flow of ions via external stimulation (i.e., light, voltage, pH, magnetic field, and temperature). These ion nanochannels, usually constructed with intrinsic or guest functionalities that are responsive to environmental simulation, drive the opening and closing of the channels. However, the gating performances of such nanoscale ion channels (i.e., gating ratios usually between 1 and 30) are far below those of BICs, due to the relatively larger nanopores in AICs, which cannot entirely block ion transport in the off states. Over the past decade, emerging advanced materials (i.e., 1D nanotubes, 2D nanosheets, and 1D-3D sub-nanoporous frameworks) with intrinsic sub-nanometer pores and stimuli-responsive properties have provided promising tools to fabricate responsive sub-nanofluidic channels with efficient gating performance. These AICs are remarkably comparable to their biological counterparts, because their more confined spaces enable a more effective closed state of the channels. Our team has developed a series of responsive sub-nanofluidic channels based on metal–organic frameworks, covalent organic frameworks, and 2D nanosheets. These sub-nanofluidic channels exhibit much higher on–off gating ratios than nanofluidic channels do, and the gating effects can be maintained over a wide range of ionic concentrations. Moreover, sub-nanofluidic channels also show stimuli-tunable ion selectivity and ion blockage effects.

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IL104 Tuning the microstructure of halide perovskites for better performance and stability

Fang Zeng[1], Tiebin Yang[1], Weiyu Kong[2], Yuhang Liang[1], Feng Li[1], Yuze Lvtao[1], Tao Wang[2], Bingguo Peng[2], Xudong Yang[2], Rongkun Zheng[1]*,

[1] School of Physics, The University of Sydney, Sydney NSW 2006, Australia.
[2] School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, China.
**Email:* rongkun.zheng@sydney.edu.au

Exceptional electronic and optical properties attracted great interest in halide perovskites within the last years. Because of their high absorption coefficient, low defect concentration, and long diffusion lengths, this material class is well suited for optoelectronics. Applications range from efficient light-emitting diodes and lasers to photodetectors and solar cells. In particular, solar cells with perovskites as the active material have been attracting widespread attention in the past decade since the pioneering work by Miyasaka and coworkers in 2009. Despite the huge progress, perovskite-based optoelectronics suffer from severe degradation. The major causes of the degradation are related to various external factors, such as moisture, oxygen, temperature, and UV light, as well as internal intrinsic factors such as ion migration, electromigration and surface reactions. Stabilising halide perovskite solar cells and other devices is a key issue for successful commercialisation. In this presentation, we report our work on improving the performance and stability of halide perovskites and relevant devices by calibrating their growth and tuning their microstructures.

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IL105 Electrode and interface designs towards better solid-state lithium batteries

Yijun Zhong, Chencheng Cao, Leqi Zhao, Moses Oludayo Tadé, Zongping Shao[1]*

[1]WA School of Mines: Minerals, Energy and Chemical Engineering (WASM-MECE), Curtin University, Perth, WA 6102, Australia
**Email: zongping.shao@curtin.edu.au*

The development of new electric applications powered by lithium(-ion) batteries could further take advantage of the abundant lithium resources in Australia. Utilizing solid-state electrolytes addresses the safety concerns associated with flammable organic liquid electrolytes in conventional lithium(-ion) batteries. Solid-state electrolytes with wide stable voltage windows are compatible with metallic lithium anode which enhances the energy density of the batteries. High resistance and instability of the interfaces on both the cathode and the anode sides are key challenges of solid-state lithium batteries. Recently, we dedicated to addressing these challenges focusing on designing new composite electrodes. These designs effectively lowered the resistances and improved the performance of the batteries. We will present our recent works on the development of lithium-containing composite anodes with functional components (e.g., Prussian blue derived dual conductive phases and titanium-based optimizers),[1-3] which focused on establishing efficient ionic and electronic pathways within electrodes and on the electrode-electrolyte interfaces for lowering overpotentials of the anode. We will also share our latest results on the composite cathodes (e.g., elemental sulfur) which focus on enhancing the utility and stability of the active cathode materials by the optimization of ionic conductive structures with functional catalysts or stabilizers.

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ABSTRACTS FROM ORAL LECTURES(OL)

OL01	**Dr. Mariam Ameen**	**RMIT University**
OL02	**Dr. Alexander Corletto**	**The University of Melbourne**
OL03	**Dr. Daqin Guan**	**Curtin University**
OL04	**Dr. Mingyu Han**	**CSIRO**
OL05	**Dr. Yueqi Kong**	**The University of Queensland**
OL06	**Dr. Vaishnavi Krishnamurthi**	**RMIT University**
OL07	**Dr. Faezeh Makhlooghiazad**	**Deakin University**
OL08	**Dr. Dan Yang**	**RMIT University**
OL09	**Dr. Shilin Zhang**	**The University of Adelaide**
OL10	**Dr. Jinqiang Zhang**	**The University of Adelaide**

OL01 Unique liquid metal activation pathways with applications for renewable transportation fuel additives and hydrogen production

Mariam Ameen, [1]* **Muhammad Mujtaba Judd**y[1], **Fahad Jabbar**[1], **Mehmood Irfan**[1], **Pierre Vaillant**[1], **Caiden Parker**[1], **Karma Zuraqi**[1], **Dan yang**[1], **Torben Daeneke**[1], **Ken Chiang**[1]

[1] *School of Engineering, RMIT University, Melbourne, VIC 3001, Australia*
**Email: mariam.ameen@rmit.edu.au*

Post-transition-based liquid metals are promising catalysts due to their high reaction rates, excellent deactivation resistance, and tuning potential, which form intermetallic and interfacial compounds through alloying with noble and transition metals.[1, 2]. The mechanism by which alloyed metals enhance activity is currently unknown and debated, with some suggesting they act as single atom catalysts[3] and others activating the liquid metal particularly gallium[4].
In the present work, Cu was incorporated into liquid Ga and EGaIn *via* a newly developed ball-milling method and tested for its catalytic behavior in a series of organic and inorganic reduction reactions. The morphology of the synthesized alloys was studied using SEM analysis while the interface was examined using XPS. These surface studies revealed that the Cu was evenly distributed in E-GaIn alloys in contrast to Ga based liquid metal alloys which were less uniform. The alloy's reactivity was evaluated through reduction reactions, including iodine-based color-change and sacrificial hydrogen production. Results showed Cu:EGaIn and Cu:Ga as mild reducing agents, useful in acetone organic condensation and glycerol acetalization to solketal, a valuable fuel additive. Detailed analysis revealed that the alloyed Cu catalyzes the oxidation of Ga present in the liquid metals. While the gallium is being oxidized in the studied scenarios, the findings lend support to the hypothesis that small amounts of alloyed transition metals can activate the gallium atoms present in liquid metal, rather than only acting as a single atom catalyst. Finally, the open circuit potential of Cu-EGaIn was measured and found to be -0.298 V vs Ag/AgCl, which is comparable to the reduction potentials of $NaBH_4$ (-0.4V) and $LiAlH_4$ (-0.34), showcasing that Cu activated gallium alloys can act as a mild reducing agent in organic synthesis, overcoming some limitations of metal hydrides while offering a milder reduction potential and heavy metal free alternative to mercury amalgams.

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OL02 Wafer-scale fabrication of black phosphorous films for infrared photodetectors

Alexander Corletto,[1] Purevlkham Myagmarsereejid,[2] Shifan Wang,[1] Wei Yan,[1] Munkhbayar Batmunkh,[2] and James Bullock[1]

1 Department of Electrical and Electronic Engineering, The University of Melbourne, Victoria, Australia

2 Queensland Micro- and Nanotechnology Centre, School of Environment and Science, Griffith University, Queensland, Australia

Email: AC: alexander.corletto@unimelb.edu.au JB: james.bullock@unimelb.edu.au

Bulk black phosphorous (bP) exhibits excellent infrared (IR) optoelectronic properties. However, most reported bP IR photodetectors are fabricated from single exfoliated flakes with lateral sizes of < 100 μm.[1, 2] Here, we fabricate wafer-scalable thin films of bP through solution deposition methods to fabricate bP IR photodetectors. To achieve this, bulk bP is electrochemically-exfoliated and a bP dispersion is prepared with laterally large bP flakes (>5 μm) that are formed into scalable thin films and applied over interdigitated electrodes to create photoconductors (Figure 1a). The bP film properties and protective capping layers were optimised to fabricate bP film photoconductors exhibiting responsivities up to 80 mA/W with 15 μs response times (Figure 1b-c) under $\lambda = 2.2$ μm wavelength illumination. The scalability of the bP thin film fabrication was demonstrated by fabricating a linear array of 25 bP thin film photoconductors on the same substrate and obtaining 25 × 25 pixel IR images with the bP linear array (Figure 1d). This research demonstrates a commercially viable method of fabricating wafer-scale BP thin films for optoelectronic devices including room temperature-operable IR photodetector arrays. A publication is currently in preparation/under review to report this research.

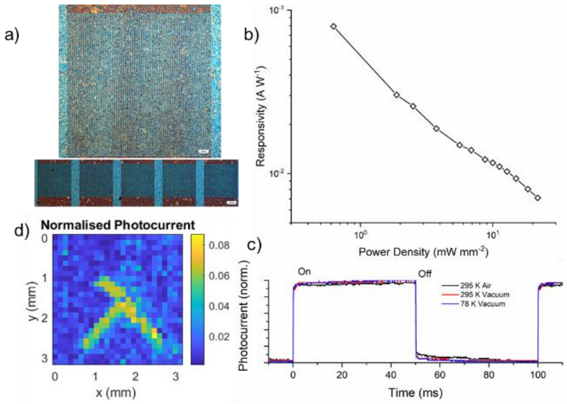

Figure 1. a) Optical microscope images of the bP thin film IR photodetectors. **b)** Responsivity of bP IR photoconductor under varying $\lambda = 2.2$ μm wavelength light power density. **c)** Photodetector response to modulated $\lambda = 2.2$ μm illumination under different environmental conditions. **d)** 25 × 25 pixel image obtained of $\lambda = 1.5$ μm wavelength light through an aperture of 'λ' symbol. Image taken using the 25-device linear array of bP thin film IR photodetectors.

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OL03 Identifying a universal activity descriptor and a unifying mechanism concept on perovskite oxides for green hydrogen production

Daqin Guan,[1,2*], Zongping Shao,[1*]

[1] WA School of Mines: Minerals, Energy and Chemical Engineering, Curtin University, Perth, Western Australia 6845, Australia.
[2] Department of Building and Real Estate, Research Institute for Sustainable Urban Development (RISUD) and Research Institute for Smart Energy (RISE), The Hong Kong Polytechnic University, Hung Hom, Kowloon 999077, Hong Kong, China.
**Email: daqin.guan@curtin.edu.au*

Producing indispensable hydrogen and oxygen for social development via water electrolysis shows more prospects than other technologies. Although electrocatalysts have been explored for centuries, a universal activity descriptor for both hydrogen-evolving (HER) and oxygen-evolving reactions (OER) has not been developed. Moreover, a unifying concept has not been established to simultaneously understand HER/OER mechanisms. Here, we rationally bridge the relationships between HER/OER activities in three common electrolytes and over 10 representative material properties on 12 3*d*-metal-based model oxides through statistical methodologies. Orbital charge-transfer energy (Δ) can serve as an ideal universal descriptor, where a neither too large nor too small Δ (~1 eV) with optimal electron-cloud density around Fermi level affords the best activities, fulfilling Sabatier's principle. Systematic experiments and computations unravel that pristine oxide with $\Delta \approx 1$ eV possesses metal-like high-valence configurations and active lattice-oxygen sites to help adsorb key protons in HER and induce lattice-oxygen participation in OER, respectively. After reactions, partially generated metals in HER and high-valence hydroxides in OER dominate proton adsorption and couple with pristine lattice-oxygen activation, respectively. These can be successfully rationalized by the unifying orbital charge-transfer theory. This work provides the foundation of rational material design and mechanism understanding for many potential applications.

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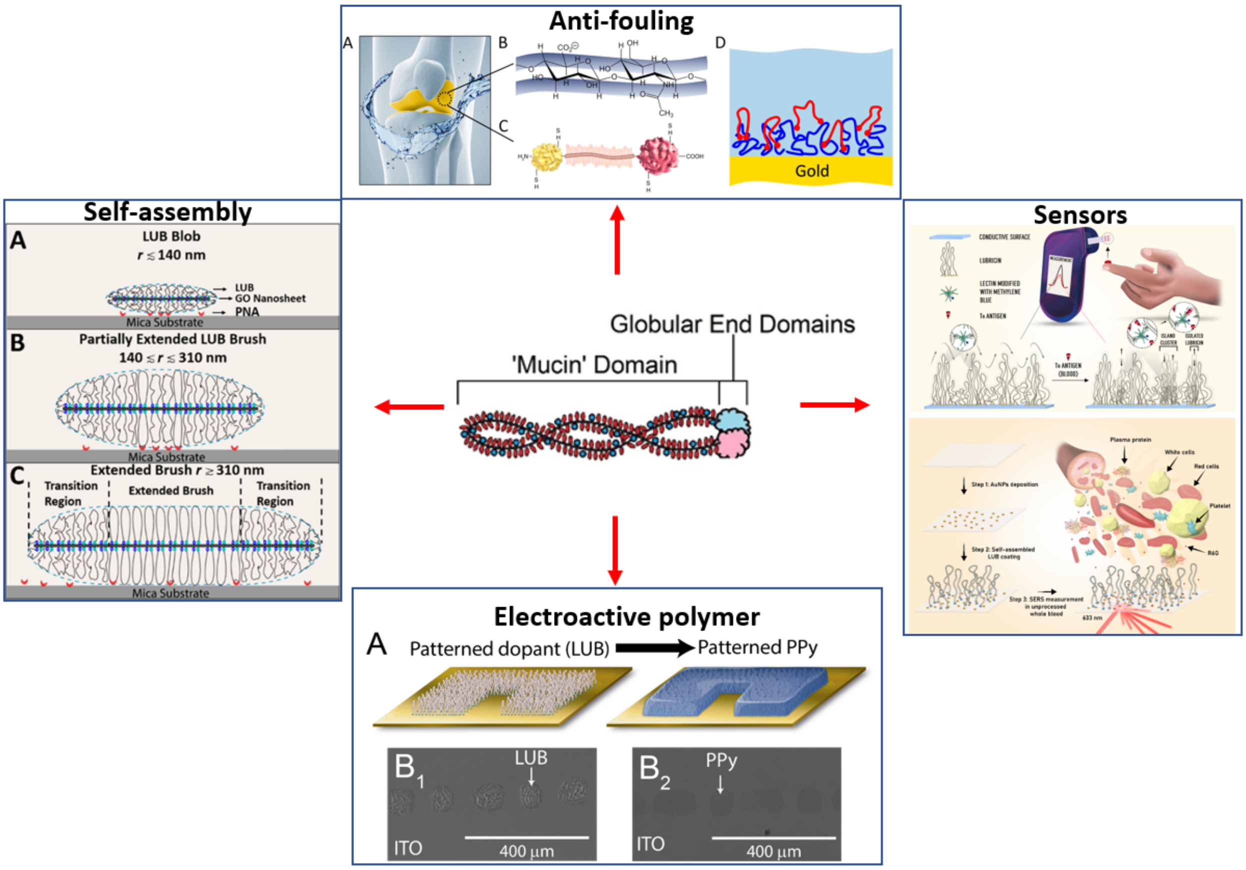
OL04 Multifunctional interfaces inspired by the self-assembled lubricin

Mingyu Han Oral Presentation[1*]

[1] *Commonwealth Scientific and Industrial Research Organization (CSIRO), Agriculture and Food, 671 Sneydes Road, Werribee, Victoria, 3030, Australia.*
**Email: mingyu.han@csiro.au*

Lubricin (LUB) is a tri-block structured glycoprotein that plays an important role as a boundary lubricant and wear protection in the synovial fluid of articular joints. In the last decade, more impressive properties of Lubricin such as interfacial self-assembly, anti-fouling, size-selective transport, high electrostatic charge density, and universal solid surface adsorption capacity without any surface modification or surface engineering have been discovered. Here we highlight several recently developed lubricin-enabled technologies applied to a diverse range of problems including improving the sensitivity and longevity of bionic neural interfaces, electrochemical and optical sensing within complex, highly fouling media (e.g. unprocessed whole blood, undiluted milk), improving the stability of 2D-nanomaterial suspensions and 2D-nanomaetials based nano-lubricant, and the fabrication of advanced electroactive polymer films.



OL05 High-capacity organic cathode materials for aluminium-ion batteries

Yueqi Kong[1], Cheng Tang[2]* , Chang Lei [1], Ashok K. Nanjundan [1], Shuimei Chen [1], Nashaat Ahmed [1], Dmitrii Rakov [1], Aijun Du [2], Xiaodan Huang[1]* , Chengzhong Yu[1]*

[1] Australian Institute of Bioengineering and Nanotechnology
The University of Queensland, St Lucia, QLD 4072, Queensland
[2] School of Chemistry and Physics
Queensland University of Technology, Gardens Point Campus, QLD 4001, Queensland

**Email:* c.yu@uq.edu.au, x.huang@uq.edu.au, c21.tang@qut.edu.au

Aluminium-ion Batteries (AIBs) are an appealing new type of battery technology with distinctive advantages such as high anode capacity, low cost and operation safety.[1] The cathode materials chosen for charge storage play a crucial role in determining the capacity and voltage of AIBs. Recently, organic materials with chemical diversity become increasingly attractive as electrodes in various battery types. P-type organic cathodes (p-OCs) such as polycyclic aromatic hydrocarbons (PAHs) undergo oxidation to form positively charged radical cations and bind $AlCl_4^-$ anions. P-OCs displayed high redox potential (> 1.5 V), which are favourable for high-performance AIBs. Despite several recent efforts on p-OCs[2], experimental studies only reached numerically one or less than one-electron redox reactions and thus relatively low specific capacities of ~70-150 mAh g^{-1}. The underlying reason for this gap is not fully revealed in the literature. It remains challenging to design p-OCs with two-electron redox chemistry and high specific capacity for AIBs.

Herein, we report a compromised electron-donating substitution strategy to excite 1-aminopyrene (ANP), a pyrene (Pyr) derivative, to undergo two-electron transfer, achieving a high specific capacity of 212 mA g^{-1} and excellent rate/long cycling performances (e.g., 106 mAh g^{-1} at 10 A g^{-1} for 12,000 cycles), superior over reported organic AIB cathodes. The electronic and steric effects of substitutes in a variety of Pyr derivatives on their functionality have been revealed. The electron-donating effect of the amino group plays two different roles, one in favoring the electron removal of neutral Pyr derivatives, another in reducing the positive charge density of oxidized radical cations. Collectively, ANP with the compromised electron-donating effect exhibits the highest binding energy with $AlCl_4^-$ and reasonable voltage within the electrolyte working threshold, enabling the unprecedented two-electron transfer.

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OL06 Fundamentals of liquid metals and alloys

Vaishnavi Krishnamurthi, [1*], Pierre Vaillant[2], Jitendra Mata[3], Caiden J.Parker[1], Salvy P Russo[4], Andrew J.Christofferson[2], Torben Daeneke[1*] and Aaron Elbourne[2*]

[1] *School of Engineering, RMIT University, Victoria, Australia*
[2] *School of Science, RMIT University, Victoria, Australia*
[3] *Australian Centre for neutron Scattering, ANSTO, NSW, Australia*
[4] *ARC Centre of Excellence in Exciton Science, School of Science, RMIT University, Victoria, Australia*
**Email: vaishnavi.krishnamurthi@rmit.edu.au*

Liquid metal systems are a new and exciting frontier in chemistry[1]. Room temperature liquid metals (RTLMs) have great potential in electronic, catalytic, and biomedical applications.[2] However, their complete utilization is hindered due to the lack of analytical techniques which can prove their bulk-liquid chemical processes. The main obstacle to studying these systems is the presence of their metallic bonds, which renders them opaque to most traditional solvent characterization techniques - as such, failing to provide atomic-level insights. Studying the nanoscale structures of liquid metals can reveal valuable information for potential applications. Neutron scattering techniques, including small angle and ultra-small angle scattering (SANS and USANS) techniques, have matured significantly in recent years and can now resolve atomic structures, clusters, and covalent associations within soft matter systems[3]. Moreover, neutrons are highly penetrative particles, meaning that they are not readily adsorbed or reflected by the liquid metal matrix, providing an avenue for experimental investigation. In this work, we provide a holistic look at the atomic arrangements of various liquid metal systems through neutron interaction using ANSTO's *Quokka* SANS for the first time. Specifically, we investigate gallium, and several gallium-based alloys, such as Cu, Bi, Zn, Sn and, In as the dopant at varying concentrations to probe the nanoscale structures of these systems, and develop structure-property relationships for RTLM systems. In the absence of deuteration, alloyed metals with substantially different scattering length densities (SLDs) are used as atomic probes to interrogate structural differences between systems. We use SANS to analyze nanoscale structures and examine changes in scattering parameters like intensity, gyration, and polydispersity. We also use a shape model to study particle interactions and aggregation. Additionally, we investigate the impact of dopant and concentration on liquid metal network ordering. DSC and MD simulations complement our SANS findings.

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OL07 Physicochemical and electrochemical properties of novel solid-state electrolytes for alkali metal batteries

Faezeh Makhlooghiazad[1], Luke A. O'Dell[1], Maria Forsyth[1] and Jennifer M. Pringle[1]
[1] Institute for Frontier Materials, ARC Training Centre in Future Energy Storage Technologies, Deakin University, Burwood, Victoria, Australia
f.makhlooghiazad@deakin.edu.au

Organic ionic plastic crystals (OIPCs) mixed with Li or Na salts have been used as electrolytes in electrochemical devices with lithium (Li) or sodium (Na) metals. OIPCs are structurally disordered solids that can possess a high concentration of vacancies within their structure that can encourage fast target ion conduction. However, the ions within the matrix of OIPC can compete with the target ion (Li+) migration under potential gradient, which may affect device performance. One approach to suppressing the migration of the matrix OIPC ions is tethering the cations and anions to produce zwitterions.

Zwitterions are a class of materials that contain covalently bonded positive and negative charges. They are non-volatile with thermal and electrochemical stability comparable with OIPCs. They have been used as additives to enhance the lithium-ion dissociation within the electrolyte systems. However, their applications as a sole matrix electrolyte in electrochemical devices have yet to be explored. Here, we have characterized the thermal, morphological and structural properties of novel zwitterions using techniques including differential scanning calorimetry, scanning electron microscopy, solid-state nuclear magnetic resonance (NMR) and electrochemical impedance spectroscopy (EIS). We used the most promising zwitterion to demonstrate their potential application as an electrolyte for Li- metal batteries. Three initial approaches have been used to demonstrate the breadth of scope of this material family: (1) plastic zwitterions can be used as the matrix material to provide a non-volatile, ionically conductive solid medium without competing ion transport; (2) the zwitterions can be used in composites with functional additives such as lithium-functionalized polymers to increase target ion transport and mechanical properties; and (3) for high-concentration electrolyte systems, the zwitterion can be combined with a high concentration of lithium salt to form a non-volatile liquid electrolyte with high lithium ion transport. Stable cycling of lithium metal cells has been achieved.[1]

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OL08 Liquid metal catalysts for direct alcohol fuel cells

Dan Yang[1]*, Pajaree Aukarasereenont[1], Muhammad Hamza Nazir[1], Ken Chiang[1], Torben Daeneke[1]

[1] School of Engineering, RMIT University, Melbourne, Australia
**Email: dan.yang@rmit.edu.au*

The direct alcohol fuel cell (DAFC) is an emerging technology that can convert the chemical energy of alcohols, e.g., methanol, ethanol, glycerol etc, directly into electricity without causing any pollutant emissions. However, their practical application is hindered by the low energy efficiency and short cycle life, which is associated with the use of expensive noble metal electrocatalysts that deactivate rapidly during cell operation. Herein, we have developed a novel bifunctional electrocatalyst based on the liquid metal, i.e., gallium (Ga). As an emerging catalytic material featured with its liquid nature, Ga can serve as both support and co-catalyst, to promote atomic dispersion of noble metals and prevent adsorption of poisonous intermediates onto the catalyst surface [1][2]. In this way, the noble metal usage can be reduced while the lifetime of catalyst can be prolonged. We have systematically investigated the composition of the alloys (i.e., type and concentration of noble metals), the reaction temperatures and the formulation of the electrolytes to optimize the activity and stability of the electrocatalysts. In particular, the liquid metal alloyed with a low concentration of noble metals, e.g., Pt (0.5 wt%)/Ga, have shown remarkable activity and stability towards both ethanol electrooxidation and oxygen reduction reaction, rendering them highly promising for the next-generation high-efficiency DAFCs.

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OL09 High entropy alloy enables efficient CO2 redox reactions

Shilin Zhang, Liang Sun, and Zaiping Guo
[1]*School of Chemical Engineering, The University of Adelaide*
Email: Zaiping.guo@adelaide.edu.au

Abstract: The performance and cyclability of lithium-CO_2 (Li-CO_2) batteries have been limited by high overpotentials and low discharge capacities. Here, we report the development of a high entropy alloy (HEA) as a novel cathode material for Li-CO_2 batteries. The HEA is composed of five metals with high mixing enthalpy and configurational entropy, leading to enhanced electrochemical activity and stability. Our results show that the HEA cathode significantly reduces the overpotential of Li-CO_2 battery and improves its long-term cyclability over 2000 hours. The excellent electrochemical performance of the HEA cathode is attributed to its high electrochemical surface area, porous structure, and enhanced catalytic activity towards CO_2 redox reaction. This work provides a promising strategy for developing high-performance cathode materials for Li-CO_2 batteries, and opens up new avenues for the design of HEA-based materials for energy storage applications.

OL10 Photothermal catalytic technology for solar fuels production

Jinqiang Zhang[1]*, Hongqi Sun[2], Shaobin Wang[1]*

[1]School of Chemical Engineering, The University of Adelaide, Adelaide, SA 5005, Australia
[2]School of Molecular Sciences, The University of Western Australia, 35 Stirling Highway, Perth, WA 6009, Australia
**Email: jinqiang.zhang@adelaide.edu.au; shaobin.wang@adelaide.edu.au*

Photothermal catalysis has recently been proposed as a promising alternative to conventional photocatalysis and thermocatalysis in the fields of energy preparation and environmental remediation, attributing to the unprecedented light harvesting efficiency, superior throughputs and moderate reaction conditions. Photothermal catalysis is basically a multiple energy complementary technology integrating solar energy mediated photochemical process and solar light induced thermocatalysis in one unit. Specifically, the photo-excited energetic hot carriers via intraband or interband extinction (also called Landau damping) can directly initiate chemical reactions in much milder conditions. And the hot carriers failing to participate the redox reactions will be converted into heat by thermalisation (also named Ohmic damping). The photo-excited hot carriers can reduce the reaction barrier and improve the reaction selectivity, while the photo-generated internal heat can thermodynamically accelerate reaction rates and ginger up the sluggish hot carriers. Therefore, photothermal catalysis has compensated the disadvantages of photocatalysis and thermocatalysis, and significantly boosted the reaction rates to a level of industrialization by taking advantage of full-spectrum solar light, showing significant potentials on large-scale production of solar fuels. Here, we present our ongoing researches in harnessing the full spectrum solar energy using the photothermal catalytic strategy to drive CO_2 reduction with alkane or hydrogen. Using solar energy to catalytically reduce CO_2 and upgrade conventional fossil fuels has the potential to convert the waste of CO_2 into high value-added chemical fuels and feedstocks in a clean and sustainable manner, allowing the dual opportunity to store the intermittent renewable energy as well as closing the anthropogenic carbon cycle.

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ABSTRACTS FROM ECR FLASH TALK

EFT01	Maryam Adavoudi Jolfaei	University of Wollongong
EFT02	Olia Alijanpourtolouti	Murdoch University
EFT03	Sandani Amanda Ekanayake	RMIT University
EFT04	Blake Armstrong	Curtin University
EFT05	Tanika Duivenvoorden	The University of Queensland
EFT06	Ziheng Feng	University of New South Wales
EFT07	Ekyu Han	The University of Queensland
EFT08	Owen Horoch	Murdoch University
EFT09	Alvin Jenner Walisinghe	Curtin University
EFT10	Wenzhong Ji	Australian National University
EFT11	Jiyun Kim	University of New South Wales
EFT12	Haritha Kirla	Murdoch University
EFT13	Tiexin Li	Curtin University
EFT14	Tamsyn Lovass	Australian National University
EFT15	Preetham Permude	Australian National University
EFT16	Shahrzad Rezvani-Baboli	Macquarie University
EFT17	Muhammad Shaharyar	Deakin University
EFT18	Mingli Tan	Australian National University
EFT19	Hengyue Xu	Tsinghua University
EFT20	Hang Yin	Australian National University
EFT21	Jierui Zhang	University of New South Wales
EFT22	Leqi Zhao	Curtin University
EFT23	Chaoyue Zhao	Deakin University

EFT01 Superfast large-size hydrogel actuators

Maryam Adavoudi Jolfaei [1], Geoffrey M. Spinks[1] * and Zhen Jiang[1] *

[1] *School of Mechanical, Materials Mechatronic, and Biomedical Engineering*

**Email: maj149@uowmail.edu.au*
gspinks@uow.edu.au
zjiang@uow.edu.au

Hydrogel actuators displaying programmable shape transformations promise to be core components in future biomedical and soft robotic devices [1]. Various approaches have been developed to increase the actuation rate such as freeze-thaw, three-dimensional printing, controlled evaporation of pre-gel solution, hydrothermal process, and electrospinning [2]. However, in these examples, the fast actuation has only been demonstrated in small-size thin films and fibers.

In our work, we overcome such challenge by presenting a facile method to generate macroporous structures in hydrogel actuators through irreversible sol−gel transition. Key to our design is the introduction of coordinate ions into thermoresponsive polymers showing lower critical solution temperature (LCST). Dehydration of thermoresponsive polymers above LCST expels water which is trapped in the pore by micro syneresis. The microstructure, thermosensivity, and mechanical properties of our hydrogels have been studied. We demonstrate that our hydrogel with a thickness of 1 cm can exhibit a high actuation speed of 1 s upon increasing the temperature above the LCST.

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EFT02 Synthesis of mesoporous silica nanoparticles with specific features for drug delivery in brain disorders

Seyedeholia Alijanpourtolouti[1]*, David J. Henry[1], Gamini Senanayake[1], Eddy Poinern[1], Sulev Koks[2]

[1] Chemistry and Physics, Murdoch University
[2] Centre for Molecular Medicine and Innovative Therapeutics, Murdoch University
**Email: olia.alijanpourtolouti@murdoch.edu.au*

Brain disorders such as Alzheimer's disease (AD) slowly destroy cells associated with memory and thinking skills and, eventually make it difficult to carry out the simplest tasks. Gene therapy offers the promise of an effective cure for both genetic and acquired brain disorders. The complexity of the blood-brain barrier (BBB) inhibits the passage of many substances including therapeutic agents from the blood to brain cells, making treatment of AD difficult [1]. Mesoporous silica nanoparticles (MSNPs) may provide a means to overcome this obstacle and transport therapeutic agents into damaged brain cells. Spherical MSNPs < 100nm have a high chance of crossing the BBB [2]. Functionalization of MSNP surfaces modifies their reactivity, enhancing biocompatibility, altering biodistribution and excretion, and elongating in vivo circulation. Previous studies have shown that negatively charged MSNPs can successfully penetrate the BBB [3]. On the other hand, positively charged MSNPs can better adsorb nucleic acids (genes) [4]. Therefore, modulating the surface charge of MSNPs will be required for the successful delivery of AD therapeutics. The pore size of MSNPs is another crucial factor that determines the adsorption of diverse therapeutical agents and the rate of their release [5]. MSNPs with pore sizes > 10 nm can encapsulate various biomolecules (protein, enzymes, and genetic molecules). This study focuses on the synthesis of mesoporous silica nanoparticles with specific features for gene delivery in brain disorders.

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EFT03 Synthesis of magnéli phase titanium suboxides and their role as efficient photothermal materials in solar steam generation

S. Amanda Ekanayake[1*], Haoxin Mai[1], Aaron Seeber[2], Sanje Mahasivam[3], Daksh Shah[1], Junlin Lu[4], Xiaoming Wen[1,4], Nishanthini Sampath[5], Nicholas Cox[5], Simon L. Schumann[6], Dehong Chen[1], Rachel A. Caruso[1]

[1]*Applied Chemistry and Environmental Science, School of Science, STEM college, RMIT University, Melbourne, Victoria 3000, Australia*
[2]*CSIRO Manufacturing 36 Gardiner Road, Clayton, VIC 3168, Australia*
[3]*Ian Potter NanoBioSensing Facility, NanoBiotechnology Research Laboratory, School of Science, RMIT University, Melbourne, Victoria 3001, Australia*
[4]*School of Science, Computing and Engineering Technologies, Swinburne University of Technology, Hawthorn, Victoria 3122, Australia*
[5]*Research School of Chemistry, Australian National University, Acton, ACT, 2601 Australia*
[6]*TU Dortmund University, Department of Chemistry and Chemical Biology, Otto Hahn-Strasse 6, 44227 Dortmund, Germany*

**Email: s3822273@student.rmit.edu.au*

Introduction of defects into the lattice structure of TiO_2 offers a versatile platform for manipulating its physicochemical and surface properties, expanding its applicability in various fields. High temperature annealing creates regular oxygen vacancy planar defects in the crystal structure of TiO_2, forming reduced titanium oxides. Magnéli phases are such substoichiometric titanium oxides which follow the formula Ti_nO_{2n-1}, with $4 \leq n \leq 9$. This work introduces a novel, cost-effective and safe carbothermal reduction method for synthesising Magnéli phase titanium suboxides, eliminating the need for TiO_2 precursor pre-treatment. Additionally, the study monitored the generation of various Magnéli phases as a function of treatment time under controlled oxygen conditions. The changes in defect stoichiometry of these carbothermally reduced titanium suboxides were analysed in depth, with a focus on their surface, bulk, optical, charge transfer, thermal, and electrical properties. This in-depth characterisation showed that multiphase Magnéli titania showed broadband light absorbance across the visible-NIR region coupled with narrow bandgaps, primarily attributed to the presence of bulk Ti^{3+} defects. The exceptional optical absorption property of Magnéli phase titanium suboxides was harnessed in solar steam generation, serving as the photothermal material, incorporated into a low thermally conductive, lightweight graphene oxide aerogel. We explored the solar steam generation performance of Magneli phases generated under various treatment times, aiming to correlate their performance with thermoelectric properties. The optimised composite exhibited an impressive energy conversion efficiency of 56%, three times higher than pure water, indicating its strong potential as a photothermal material for solar energy conversion applications.

EFT04 MuStaRD: A general utility program for multi-state reactive descriptions using empirical valence bond theory

Blake I. Armstrong[1]*, Luc LeBlanc[1], Paolo Raiteri[1], Julian D. Gale[1]

[1] *School of Molecular and Life Sciences, Curtin University, Perth (WA), Australia*
**Email: blake.armstrong@postgrad.curtin.edu.au*

The study of chemical reactions typically involves the formation and/or breaking of chemical bonds, or the migration of electrons, with an associated activation barrier. For instance, modelling reactivity is necessary in the study of proton-conducting solid oxide fuel cells [1] and ion conducting cathode materials within batteries [2]. When attempting to study the dynamics of these processes theoretically in systems with many particles over meaningful timescales *ab initio* quantum mechanical and hybrid quantum-mechanical/molecular mechanics methods can become computationally expensive and impractical. On the other hand, classical force field methods offer the expediency required to perform these tasks but are usually limited to the examination of near-equilibrium processes and are incapable of handling chemical reactivity. Some notable exceptions include reactive force fields [3], which have been useful in studying a multitude of chemical reactions but require extensive expertise to construct and parameterise; and other methods [4] which can enable bond dissociation but are unable to describe bond formation or reaction barriers.

An alternate approach to enable the description of reactivity starting from conventional unreactive force fields is that of empirical valence bond (EVB) theory [5]. EVB theory enables unreactive force fields, each describing separate potential energy surfaces, to be mixed in a controlled way to describe intermediate reaction states in a chemical reaction.

There are several codes in which EVB theory has been implemented [1,6], which are largely developed to suit a particular field of interest, or are not open-source and cannot be modified/verified. Here we present a new open-source generalised implementation designed to be modifiable and extensible while remaining applicable to a wide set of chemical reactions. The program is written in Python and utilises LAMMPS as the main MD engine through its Python API. The implementation has been verified against previous EVB simulations of proton diffusion through a crystal of $BaZrO_3$ [1], successfully reproducing the diffusion coefficient at various temperatures.

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EFT05 Calculating ionic conductivity of electrolytes for magnesium batteries

Tanika Duivenvoorden,[1]* Stephen Sanderson,[1] Debra Searles[1,2]

[1] *Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Qld, Australia*
[2] *School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Qld, Australia*
**Email: t.duivenvoorden@uq.edu.au*

Improving battery technologies for energy storage is vital to the transition from fossil fuels to more sustainable energy, due to the variable nature of renewables such as wind and solar power. Conventional Li-ion batteries use flammable organic electrolytes and have limitations in sustainability due to the low abundance of lithium in the earth's crust. [1] Magnesium batteries are an attractive solution for safer and more sustainable energy storage, as magnesium is cheap, abundant, non-toxic, and non-dendritic. [1, 2] Standard electrolytes composed of flammable organic liquids are not compatible with the magnesium anode, and safer alternatives such as solid-state or aqueous electrolytes are being investigated. [2] An important concept in the development of these alternatives is the ionic conductivity and diffusion of magnesium ions through the material. These transport phenomena can be observed in detail using molecular simulations, which offer atomic-level information on the transport mechanisms to inform the development of improved electrolyte systems. This work explored different methods of running non-equilibrium molecular dynamics (NEMD) simulations to calculate the ionic conductivity and diffusion coefficients of an aqueous $MgCl_2$ electrolyte. Using NEMD methods, the Mg^{2+} ion conductivity and diffusion coefficient were also calculated in a solid-polymer polyethylene glycol and $MgCl_2$ electrolyte system. This method can be used to investigate the ionic conductivity of a range of different electrolytes, and future work will aim to assess alternative solid-polymer matrices and different magnesium counterions.

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EFT06 A self-rechargeable moist-electric generator with diverse applicable conditions

Ziheng Feng[1*], Chao Liu[1], Renbo Zhu[1], Shuo Zhang[1], Tao Wan[1*], Dewei Chu[1]

[1] *School of Materials Science and Engineering*
UNSW, Sydney NSW 2052
**Email: ziheng.feng@student.unsw.edu.au*

71% of the Earth's surface is covered by water[1] and harvesting energy from water has recently become an emerging topic in the development of sustainable energy[2-4]. As a derivative of water, moisture, which exists world widely, possesses higher internal energy than other forms of water. This unique characteristic significantly endows moisture a great potential to be studied as an energy source. With this aid, moist-electric generators (MEGs) are proposed as prototypes to convert energy from moisture[5, 6]. Despite the substantial achievement in output performance, the existing MEGs are commonly restricted to application in high-humid and mild-temp regions, which certainly hampers their widespread commercially[7]. Hydrogel intrinsically possesses water like a "reservoir", whose function is tailorable by mixing with different materials[8, 9]. Therefore, the adoption of hydrogel in MEGs is of great interest to be explored. Herein, we have developed a hydrogel-based MEG (HMEG) that is capable of working continuously at the room condition (25 ℃ and relative humidity of 40%) or even in severer conditions (50 ℃ or -20 ℃). More importantly, the hydrogel displays a self-rechargeable function in compensating for the loss of the internal water content by absorbing ambient moisture, which is constructive in realizing the function of cyclic usage. Besides the outstanding current output, a high voltage output could be also easily achieved by scalable connection of multiple devices is series, which is feasible to power up different electronics (e.g., LEDs, smart window etc.).

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EFT07 High performance indoor perovskite solar cells by self-suppression of intrinsic defects via dmf-free solvent engineering

EQ Han[1], Miaoqiang Lyu[1*], Jung-Ho Yun[1,2*], Lianzhou Wang[1*]

[1] *Nanomaterials Centre, School of Chemical Engineering,*
Australian Institute for Bioengineering and Nanotechnology,
The University of Queensland (St Lucia), Brisbane, QLD 4072, Australia First Affiliation
[2] *Air & Environment Energy Nexus Lab*
Department of Environmental Science and Engineering
College of Engineering, Kyung Hee University, Gyeonggi-do 17104, Republic of Korea
**Email: ekyu.han@uq.edu.au*

Lead halide perovskite solar cells are gaining significant attention for their potential in indoor photovoltaic applications. To optimize their indoor performance, it's crucial to minimize inherent defects in the perovskite active layer. In this study, a simple solvent-engineering approach has been devised to effectively mitigate both surface and bulk defects in indoor lead halide perovskite solar cells, achieving an impressive efficiency of 35.99% under 1000 lux cool-white LED lighting. The key improvement involves substituting dimethylformamide (DMF) with N-methyl-2-pyrrolidone (NMP) as the solvent in the perovskite precursor. This replacement substantially reduces intrinsic defects within the resulting perovskite films, leading to longer charge carrier lifetimes and decreased non-radiative charge recombination in the devices. The enhanced performance can be attributed to the stronger interaction between NMP and formamidinium iodide/lead halide compared to DMF. This interaction significantly enhances the quality of the perovskite thin films, resulting in reduced interfacial halide deficiencies and non-radiative charge recombination. Overall, this research lays the foundation for the development of efficient indoor perovskite solar cells, catering to the growing demand for power sources for Internet of Things (IoT) devices.

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EFT08 Functionalised silica nanoparticles for agriculture

Owen Horoch[1]*, David Henry[1]

[1] *Murdoch University*
Email: owen.h@iinet.net.au

Micronutrient deficiencies of essential trace elements in agricultural crops lead to lower yields and less nutritious products.[1] Australian soil is notoriously lacking in micronutrients such as zinc, copper, manganese and molybdenum.[2] These deficiencies carry through to the grains grown in these soils and foods produced from these grains. Foliar fertilisers can assist in delivery of essential micronutrients to plants more efficiently than traditional soil-based fertilisers as they are applied to the plant directly, require less fertiliser and reduce run-off and leaching into waterways.[3] Nanoparticles have the potential to act as targeted delivery agents in foliar fertilisers and to fortify grains with some of these essential trace elements.[4]

Fluorescently-tagged monodisperse mesoporous silica nanoparticles (MSNs) have been functionalised with different surface coatings, added to micronutrient solutions and sprayed onto wheat plants to track the location of where the nanoparticles end up and to test the benefits of foliar application on the overall micronutrient content within the grain.

Certain surface modifications of the MSNs appear to work better than others at accumulating within the tillers of the wheat plants and moreso the grains of the plants in the early stages of flowering.

The initial findings indicate that functionalising the nanoparticles with molecules that the plants are known to utilise in biological processes enables enhanced uptake and translocation.

These findings suggest that surface modifications to MSNs with higher efficacy for delivery to the seed grain have been found.

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EFT09 Crystal shape and topography: prediction and optimisation with thecrystalgrower model

Walisinghe AJ1*, Spackman PR1, Anderson MW2, Gale JD1
1 Curtin University, Australia
2 University of Manchester, United Kingdom

**Email: alvin.walisinghe@curtin.edu.au*

Particle or crystal shape engineering represents a fundamental aspect of any industry that produces or handles solid matter, including fields such as, pharmaceuticals, agrochemicals, energy, and electronics. Numerous important physical properties, such as mechanical strength, dissolution/sublimation rates, agglomeration, and compressibility are influenced by the crystal shape. Therefore, understanding the effects of intermolecular interactions on the shape and size of a crystal becomes crucial in determining how these physical properties can be controlled.

The CrystalGrower software developed by Anderson et al. [1,2] provides a generalised Monte Carlo (MC) model for crystal growth, introducing an improved 3D approach based on the MONTY approach by Meekes and co-workers. [3] The model can be utilised to simultaneously model both the crystal shape and surface features. Those which are automatically generated and governed by the input (free) energy parameters for specified intermolecular interactions within a nearest neighbour model, obtained from a crystal structure.

The general workflow for CrystalGrower to date has involved fitting of the nearest neighbour interaction energy parameters to an experimentally observed crystal shape and information from atomic force microscopy. In this work, a powerful new automated protocol will be presented that rapidly predicts the free energies of interaction for use within such a MC model for a wide range of molecular crystalline solids and solvents, thereby removing a major bottleneck to the study of new materials. Furthermore, it will be shown how global search algorithms can also be utilised along with a robust shape descriptor and a reference (experimental) crystal shape to optimise the aforementioned interaction energies. In combination, the above methods create a powerful tool that can aid crystal shape engineering across a wide array of fields.

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EFT10 Bulk photovoltaic effect of thin batio$_3$ films integrated on silicon

Wenzhong Ji,[1]* Teng Lu,[1] Genmiao Wang,[1] Hua Chen,[1] Yun Liu,[1]

[1] Research School of Chemistry, The Australian National University, Canberra, ACT 2601, Australia.
**Email: Wenzhong.ji@anu.edu.au*

The bulk photovoltaic (BPV) effect was first discovered in materials without inversion symmetry in the 1950s and since then it has received intensive attention. Unlike conventional solar cells, it doesn't rely on interfaces like p-n junctions or Schottky barriers for charge separation, so fosters simplicity in design. For decades, many perovskites structure ferroelectric materials (FEs) have been grown on high-cost single crystal substrates to investigate their BPV performance [1]. Recently, the BPV is also utilized for memory [2] and computation [3], so integrating these FEs possessing BPV on silicon will be more feasible to combine with the current semiconductor industry. Here we successfully grow (001)-oriented barium titanate (BTO) thin films on Si using CeO_2 and yttria-stabilized zirconia (YSZ) buffer layers without removing the natural oxide layer. Because of a strong self-polarization, under 375 nm wavelength laser illumination, these films generated stable short-circuit current ~10.6 μA/cm^2 and high open-circuit voltage ~0.7 V. As a main feature of BPV, the current varies with the light polarization directions. Besides, the photocurrent linearly increases with light intensity while the photovoltage is not affected. These observations are highly consistent with the ballistic mechanism. It is believed the deposition of high crystalline BTO films on Si with significant photo response will pave a way for photoelectric devices investigation and their promising applications.

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EFT11 High-performance all-inorganic perovskite nanocrystals based no$_2$ gas sensor

Jiyun Kim[1], Chun-Ho Lin[1], Long Hu[1], Tom Wu[1]*, Dewei Chu[1]*

[1] School of Materials Science and Engineering, University of New South Wales (UNSW),
Sydney, NSW 2052, Australia
**Email: d.chu@unsw.edu.au*

Chemiresistive sensing is one of the most promising advanced technologies for a portable, flexible, and reliable sensing platform and in high demand across various applications ranging from air quality monitoring to explosive detection and medical diagnostics. Despite intense studies on improving performance of chemiresistive NO_2 sensor, the existing chemiresistive NO_2 sensors still suffer from issues such as low sensitivity, high operating temperature, slow response/recovery time. Herein, we report a high-performance NO_2 sensors based on all-inorganic perovskite nanocrystals (PNCs), achieving room temperature operation with ultra-fast response and recovery time. With varying halide composition, a superior sensitivity of ≈67 at 8 ppm NO_2 is achieved in $CsPbI_2Br$ PNCs sensors with a detection level down to 2 ppb, which outperforms other existing nanomaterial-based NO_2 sensors. Our work thus has implications for developing the next generation of gas sensing platform with point-of-care NO_2 detection technologies.

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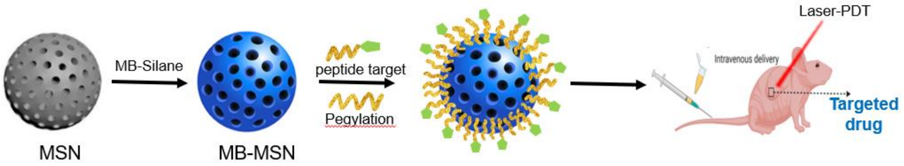
EFT12 A novel peptide targeted photodynamic therapy for triple negative breast cancer

Haritha Kirla[1,2]*, Juliana Hamzah[2], David J Henry[1]

[1]Chemistry and Physics, Murdoch University, Perth, WA, Australia
[2] Harry Perkins Institute of Medical Research, Nedlands, WA, Australia
**Email: haritha.kirla@murdoch.edu.au*

Triple negative breast cancer (TNBC) is a subtype of breast cancer that is very difficult to treat. Lately, photodynamic therapy (PDT) has been gaining interest as a therapeutic approach and appears to be a propitious alternative for treating localised breast cancers including TNBC. PDT involves light activation of a photosensitiser molecule to produce reactive oxygen species that cause destruction of cellular targets. It is a clinically approved method to treat various cancers. However, accumulation of photosensitiser molecules in tumours is not selective, resulting unwanted side effects. To overcome this, we have developed a new approach, called targeted PDT. In this work, we aimed to deliver a photosensitising drug, methylene blue (MB) precisely at the TNBC tumour site using a nanodrug formulation made of mesoporous silica nanoparticles (MSN)[1,2]. For this, we developed a novel drug formulation in which MB covalently encapsulated in MSN (MB-MSN) using our recently developed MB silane derivative[3]. Then the surface of MB-MSN was modified using a tumour homing peptide that can bind selectively to breast cancer tumour cells[4]. The results showed that MB-MSN has higher fluorescence, enhanced generation of reactive oxygen species and minimal photosensitiser leakage. Further, peptide attachment improved the target binding capability, which will potentially reduce unwanted biological interactions. In addition, particles demonstrated safety in mice. We believe this targeted PDT approach will provide a new treatment solution for treating deadly TNBC and will be translatable to clinical settings.



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EFT13 Terminal deuterium atoms protect silicon from oxidation

Tiexin Li, [1] Nadim Darwish [1]*

[1] School of Molecular and Life Sciences, Curtin University, Bentley, WA 6102, Australia
**Email: tiexin.li@postgrad.curtin.edu.au, nadim.darwish@curtin.edu.au*

In recent years, the hybrid silicon-molecular electronics technology has been gaining significant attention for applications in sensors, photovoltaics, power-generation and molecular electronics devices. However, Si–H surfaces, which are the platform on which these devices are formed, are prone to oxidation, compromising the mechanical and electronic stability of the devices. Here, we show that when hydrogen is replaced by deuterium, the Si–D surface become significantly more resistant to oxidation when either positive or negative voltages are applied to the Si surface. Si–D surfaces are more resistant to oxidation and their current–voltage characteristics are more stable than those measured on Si–H surfaces. At positive voltages, the Si–D stability appears to be related to the flat band potential of Si–D being more positive compared to Si–H surfaces, making Si–D surfaces less attractive to oxidizing OH- ions. The limited oxidation of Si–D surfaces at negative potentials is interpreted by the frequencies of the Si–D bending modes being coupled to that of the bulk Si surface phonon modes, which would make the duration of Si–D excited vibrational state significantly less than that of Si–H. The strong surface isotope effect has implications in the design of silicon-based sensing, molecular electronics and power-generation devices, and on the interpretation of charge transfer across them.

The strong isotope effect is interpreted by the frequency of the bending modes of Si–D being closer to that of the bulk Si surface phonons than Si–H. It is therefore expected that Si–D can be de-excited rapidly via the Si phonon modes. This can lead to surface bound Si–D bonds being much more resistant to desorption than Si–H, which in turn, can limit homolytic cleavage and the generation of Si radicals that initiate Si oxidation when the Si surface is negatively biased. At positive voltages, Si–D surfaces appears less attractive to oxidizing OH- ions because Si–D have a more positive flat band potential compared to that of Si–H surfaces. The strong surface isotope effects reported here have implication in the design of silicon-based devices, molecular electronics and power-generation devices based on silicon, and on the interpretation of their charge transport characteristics.

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EFT14 The synthesis, structure and properties of ferroelectric lead-based perovskite materials

Tamsyn Lovass[1*], Teng Lu[1], Felipe Kremer[2], Frank Brink[2], Yun Liu[1]

[1] Research School of Chemistry, The Australian National University, ACT, 2601
[2] Centre For Advanced Microscopy, The Australian National University, ACT, 2601
**Email:* tamsyn.lovass@anu.edu.au

Lead-based perovskite systems have been historically widely studied due to their remarkable piezoelectric and ferroelectric properties. Although these materials have are researched thoroughly for applications in devices such as SONAR, actuators, sensors and more[1], little work has been done until recently in deeply studying their structure-property relationships. Without understanding chemical and structural factors that contribute to their high performance, it is difficult to have logical strategies for modifying complex systems like PIN-PMN-PT ($Pb[Mg_wIn_xTiyNb_z]O_3$) to enhance their applicability.

This work reports the synthesis of PMN ($Pb[Mg_{1/3}Nb_{2/3}]O_3$), PT ($PbTiO_3$), and 0.75PMN-0.25PT as single-phase ceramics by conventional solid state methods. Electron diffraction patterns of the binary system PMN-PT and the ternary system PIN-PMN-PT contain information about the average and local structures induced by both the long range ordering of cations and polyhedral tilting[2]. This particularly manifests as weak transverse diffuse scattering. The local structure can be correlated with the dielectric, piezoelectric and ferroelectric properties displayed by these ceramics, providing unprecedented insight into the local structure-property correlations in the PIN-PMN-PT system, clarifying why a deep understanding of the local structure of materials is integral in future progress in materials chemistry.

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EFT15 Noble metal free transition metal oxide for hydrogenation of N-ethylcarbazole in hydrogen storage application

Preetham Permude[1*], Hua Chen[1], Terry Frankcombe[2] and Yun Liu[1]

[1] Research School of Chemistry, The Australian National University, Canberra, ACT 2601, Australia
[2]School of Science, The University of New South Wales, Canberra, ACT 2601, Australia.
**Email: Preetham.permude@anu.edu.au*

Hydrogen storage is one of the key technology which is required for the development of hydrogen economy[1]. Among various approaches for development of hydrogen storage technology, LOHC (liquid organic hydrogen storage) has advantage of easy thermal management, high hydrogen density and good compatibility with existing liquid fuel infrastructure [2]. In this regard, we report a noble metal free transition metal oxide catalyst which has not been well studied or reported for the hydrogenation of LOHC material N-ethylcarabazole (NEC). The efficiency of the NiO (nickel oxide) catalyst is enhanced by the addition of copper (Cu) into the solid solution and as the concentration of Cu increased from 1 mol% to 4 mol%, the degree of hydrogenation of NEC increased. The $Cu_{1-x}Ni_xO$ catalyst with 4 mol% Cu showed 5.45% weight % of hydrogen compared to 4.79 weight% of hydrogen of NiO. Our work proves that a noble metal-free catalyst can be used for hydrogen storage into aromatic LOHC and provides insight into designing of low-cost catalyst for this application

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EFT16 Synthesis of ruby nanoparticles with controlled optical properties for biological applications

Shahrzad Rezvani-Baboli, [1]*, Louise J Brown, [1], Alfonso E Garcia-Bennett [1]

[1] School of natural Sciences, Macquarie University, Sydney, 2109, Australia
**Email: shahrzad.rezvani-baboli@hdr.mq.edu.au*

Despite many promising advancements in the development of fluorescent probes, significant optical and chemical drawbacks still remain for using most probes for biological applications; and so, the search for a new generation of bio-probes continues. In this presentation, we describe the controlled synthesis of ruby (α-Al_2O_3:Cr^{3+}) nanoparticles. The low molar concentrations of chromium ions doped in the highly stable α-Al_2O_3 crystal creates unique optical properties in the near-infrared spectral region. We investigate the optical and physical properties of these nanoparticles, and demonstrate how these properties can be tuned by controlling the synthesis parameters. Nanoruby is particularly interesting due to its narrow emission with long lifetime and high photostability in the red region of the visible spectrum. Our results reveal the unique potential of these nanoparticles for future far-red and near-infrared bioimaging, and provide new insights into the synthesis and characterisation of advanced materials for biological applications.

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EFT17 Development of new organic ionic plastic crystal based membranes for CO_2 separation.

Muhammad Shaharyar,[1]* Douglas R. MacFarlane[2], Mega Kar,[1] Jennifer M. Pringle,[1]

[1] Institute for Frontier Materials, Deakin University, Burwood, VIC 3125, Australia.
[2] School of Chemistry, Monash University, Clayton, VIC 3800, Australia
**Email: s.shaharyar@deakin.edu.au*

There is an urgent need for the development of more efficient technologies to mitigate climate change, such as the separation and capture of CO_2 from flue gas. This work explores light gas separation based on a series of novel Organic Ionic Plastic Crystals (OIPCs) and polymer composite membranes. OIPCs have high tunability due to the presence of various cations and anions. Another important feature of OIPCs is their thermal profile marked with a solid-solid phase transition which involves structural changes and rotational modes of ions. Previously OIPCs have been shown to be a promising material for light gas separation [1]. In this study OIPCs based on different cations and fluorinated anions were co-casted with Poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP). The findings indicate that cation and anion both play an important role in the CO_2 selective uptake unlike Ionic Liquids (ILs) for which anion is primarily responsible for the CO_2 uptake. Cations having oxygen atom in their ring demonstrated higher permeability than the ones without the oxygen atom. 3,3-dimethyloxazolidinium bis(fluorosulfonyl)imide [C_1moxa] [FSI] recorded the highest selectivity ($\alpha_{CO2/N2}$ = 205) amongst others surpassing the upper bound of the Robeson plot [2]. Furthermore, substantial changes in separation performance were observed in OIPCs that underwent a solid–solid phase transition. A shift from phase II to phase I resulted in a significant increase in selectivity (from ~65 to ~ 167) for the 4-isopropyl-4-methylmorpholinium bis(fluorosulfonyl)imide [C_{i3}mmor] [FSI] based composite membrane. Analysis of the relationship between structure and transport properties of the different composites provides insights into the impact of different cations and anions, suggesting a promising new direction in the development of highly permeable and selective gas separation membranes.

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EFT18 Material properties and tunability of vinylpyridine block copolymer systems

Ming Li Tan[1]*, Qiao Yan[1], Zhen Jiang[2], John Holmes[1], John W. White[1], Zbigniew Stachurski[1], Pu Xiao[1], Yun Liu[1], Luke Connal[1]

[1] *The Australian National University*
[2] *University of Wollongong*
Email: mingli.tan@anu.edu.au

Block copolymers, composed of distinct segments with different chemical compositions, exhibit unique characteristics which arise from the spontaneous organization of their microdomains on a nanometer scale.[1, 2] This study compares the material properties and self-assembly behaviour of vinylpyridine isomers in a block copolymer system. RAFT polymerization techniques were employed to precisely control the molecular weight and chemical composition of the polymer. Advanced characterization tools such as spectroscopy, electron microscopy, and X-ray scattering techniques were utilized to explore the domain morphology. Plus, mechanical characterization tools such as Dynamic Mechanical Analysis and tensile testing was conducted to study the bulk phase properties. Most bulk phase block copolymer studies on vinylpyridine were conducted by linking vinylpyridine with another hard phase material like styrene. By combining vinylpyridine with a soft phase, self-healing properties was observed for this block copolymer system. In addition to this, this material is moisture-responsive, exhibiting an increase in fluorescence post-exposure to water.

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EFT19 Exceptional anisotropic noncovalent interactions in ultrathin nanorods: the terminal σ-hole

Hengyue Xu [1],*, Daqin Guan[2],*
[1] Tsinghua Shenzhen International Graduate School, Institute of Biopharmaceutical and Health Engineering, Tsinghua University, Shenzhen518055, China
[2] Department of Building and Real Estate, The Hong Kong Polytechnic University, Hung Hom, Kowloon999077, Hong Kong, China
**Email: xuhy21@mails.tsinghua.edu.cn, daqin.guan@polyu.edu.hk*

Nanomaterial is the Holy Grail of material science, which has been widely applied in the fields of energy, environment, chemistry, and biomedicine. Its catalytic merits were usually ascribed to the advantages of size effect, strain effect, and covalent effect. Noncovalent interactions are critical in the catalysis processes but often overlooked. Herein, different from the traditional understandings, we discover for the first time and give systematic insights into a unique noncovalent terminal σ-hole phenomenon in the 3d-metal-based nanorods, which should be one of the key origins of nanomaterial activity. As a proof-of-concept, pure metal and alloyed core–shell nanoclusters/nanorods composed of the two most important 3d metals (Co and Ni) growing from 0.5 to 2.5 nm are investigated. Unlike nanoclusters, the σ-hole only appears at the terminal sites of nanorods and the magnitude of the terminal σ-hole generally enhances with the growing processes. Further investigations show that this terminal σ-hole is closely related to the important physicochemical properties of nanorods. For example, the work function along the axis of the terminal σ-hole is smaller than other directions, contributing to the facile electronic transport along the axis of the terminal σ-hole. Most importantly, we find that the d-orbital center of the atoms around the terminal σ-hole shifts closer to the Fermi level as compared with other atoms, which can endow the terminal sites in nanorods with the higher chemical adsorption capability. We believe that this work will provide critical guidance for the rational design of nanomaterials in many potential applications.

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EFT20 Defect engineering enhances plasmonic-hot electrons exploitation for CO_2 reduction over polymeric catalysts

Hang Yin, [1]*, Zongyou Yin[1]**

[1] *Research School of Chemistry, Australian National University, ACT 2601, Australia.*
**Email: Hang.Yin@anu.ede.au*
***Email: Zongyou.Yin@anu.edu.au*

Defects play important roles in heterogeneous catalysis. The presence of defects can optimise catalytic processes by modulating adsorption properties, regulating electronic structure, tuning selectivity and enhancing activity (lowering the activation barrier) of the catalyst.[1] Accumulated evidence has shown that defect density correlates with the catalytic activity of solid catalysts, as more defects introduce more coordination sites, leading to a better reactant absorption. In addition, as the defect is usually the active sites for catalysis, the increased density of defects increases the overall reaction rate. In addition, the efficient utilisation of defects for photocatalysis however needs a sufficient electron flux. In conventional photocatalysis, these come from photoirradiation of a semiconductor substrate, which places a limitation of the rate of electron injection to active sites. An attractive alternative is to exploit the plasmonic effect, which can provide additional hot electrons to promote the photocatalytic reaction.[2] Herein, we have investigated defect engineering within a hybrid system composed of ‘‘soft’’ polymer catalysts and ‘‘hard’’ metal nanoparticles, employing the disparity in their thermal expansions. Electron paramagnetic resonance, X-ray photoelectron spectroscopy, and mechanistic studies together reveal the formation of new abundant defects and their synergistic integrability with plasmonic enhancement within the hybrid catalyst. These active defects, co-localized with plasmonic Ag nanoparticles, promote the utilization efficiency of hot electrons generated by local plasmons, thereby enhancing the CO_2 photoreduction activity while maintaining the high catalytic selectivity.[3]

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EFT21 Water harvesting using the UiO-66 metal-organic framework: Unraveling the Role of Functionalization and Defects using Computational tools

Jierui Zhang,[1]* Francesco Paesani,[2] Martina Lessio[1]

[1] *School of Chemistry, UNSW Sydney, Kensington, NSW, Australia*
[2] *Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA, USA* **Email:*
**Email: jierui.zhang@student.unsw.edu.au*

The shortage of clean water is a global concern driven by the increasing world population. Atmospheric water is a potential resource for relieving the water scarcity. However, existing atmospheric water harvesting technologies are limited by significant energy costs and high humidity requirements.[1] The UiO-66 metal-organic framework (MOF) is a promising water harvesting material due to its high stability,[2–4] large surface area,[3,5] reversible water adsorption ability[5,6] and low energy requirement for framework regeneration.[6] Thus, the employment of UiO-66 and MOFs in general in water harvesting technologies could help overcome the existing limitations, but a fundamental comprehension of the adsorption mechanism is required to scale up this technology for industrial applications.[4,7]

In this work, we provide computational insights into the adsorption mechanism of water in the UiO-66 framework. Utilising molecular dynamics (MD) simulations, we systematically explore the profound influence of functionalization and defects on this adsorption process. To achieve this, we developed force field models for pristine and defective UiO-66, as well as UiO-66-NH_2, UiO-66-OH, and UiO-66-$(OH)_2$. These models were benchmarked against ab-initio results and experimental infrared spectra. Our findings reveal μ_3-OH sites as the preferential interaction sites for water in these frameworks, and the formation of localised water clusters inside the octahedral pores is responsible for the abrupt water uptake step in experimental adsorption isotherms. Functional groups in the framework allows water to cluster in the octahedral pores at lower water loading, causing the abrupt uptake to occur at lower relative humidity. Furthermore, our preliminary results on UiO-66 with missing-linker defects reveal a distinct affinity of water towards these defect sites, which explain the experimentally observed enhanced adsorptive performance of the defective MOF.[8] Overall, the findings presented in this contribution are crucial for guiding the design and synthesis of the next-generation of water harvesting MOFs.

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EFT22 Enhanced high-temperature cycling stability of garnet-based all solid-state lithium-ion batteries by bi-functional cathode electrolyte interlayer

Leqi Zhao, Yijun Zhong, Chencheng Cao, Zongping Shao[1]*

[1]WA School of Mines: Minerals, Energy and Chemical Engineering (WASM-MECE), Curtin University, Perth, WA 6102, Australia. E-mail: zongping.shao@curtin.edu.au

Abstract

The pursuit of safer and high-performance lithium-ion batteries (LIBs) has triggered extensive research activities on solid-state batteries. However, challenges related to the unstable electrode-electrolyte interface, particularly the cathode-electrolyte interface, hinder their practical implementation. Polymer has been used extensively to improve the cathode and electrolyte interface in garnet-based all-solid-state LIBs (ASSLBs) with favorable performance at room temperature, while it introduces new concerns about thermal stability. In this study, we propose the incorporation of a bi-functional flame-retardant triphenyl phosphate (TPP) additive into a solid polymer electrolyte (SPE) of poly(ethylene oxide) (PEO), acting as a thin buffer layer between NCM cathode and garnet electrolyte. Through electrochemical stability tests, cycling performance evaluations, interfacial thermal stability analysis and flammability tests, improved thermal stability (capacity retention of 98.5% after 100 cycles) and safety characteristics (safe and stable cycling up to 100 ℃) of the modified garnet-based ASSLBs with NCM cathodes are demonstrated. Based on various material characterizations, the mechanism for the improved thermal stability of the interface is proposed. The results highlight the potential of bi-functional flame-retardant additives to address the challenges associated with the electrode-electrolyte interface in ASSLBs at high temperature, which may benefit the cycling stability of the cells at fast charging and overcharging conditions where the battery's operating temperature may obviously exceed ambient conditions. Efficient thermal modification in ASSLBs operating at elevated temperatures is also essential for enabling large-scale energy storage, with safety being the a primary concern. ***Keywords: solid-state batteries, cathode electrolyte interlayer, flame-retardant additives, cycling stability, interfacial stability, thermal stability***

The ORCID identification number(s): https://orcid.org/0000-0003-2270-1257

EFT23 Predicting Ion transport through structurally-complex graphene oxide structures

Chaoyue Zhao[1]*, Natalya A. Garcia, Joel B. Awuah, Filip Vuković, Ruitao Jin, Tiffany R. Walsh

[1]Institute for Frontier Materials, Deakin University, Geelong, VIC 3216, Australia

Email: *zhaocha@deakin.edu.au*

Graphene oxide (GO) could be a cost-effective material for water filtration and desalination. To maximize the potential of GO in this area, deeper structure/property relationships of GO need to be established, and molecular simulation is one approach to achieve this goal. However, idealized GO structures (such as those based on the Lerf-Klinowski model[1]) are commonly used in the field of molecular simulation, which do not contain holes, topological defects, etc in the GO nanostructures[2, 3]. A new computational protocol is introduced to create realistic GO sheet structures with novel complexity that can be directly applied in molecular dynamics simulations[4]. Using this procedure, structurally-complex GO membrane stacks were computationally constructed and characterized. Some aspects of the GO membrane structure were investigated such as the vertical distance between two adjacent layers (parallel to the GO membrane stacking direction, *e.g.* the interlayer spacing). In addition to this, studies of ion transport in an aqueous environment have been conducted for both a single perforated GO sheet, and a stacked bilayer of perforated GO. These studies made use of umbrella sampling simulations to estimate the free energy profile associated with single-ion transport, and subsequent studies examined spontaneous multi-ion transport for 0.6M salt solutions. The use of structurally-complex GO sheets to make GO membrane stacks resulted in highly heterogeneous interlayer spacings that could not be recovered in the case of GO membrane stacks made from LK GO sheets. This results in a more highly tortuous set of potential pathways for ion transport, more closely capturing the likely scenario in real GO membranes. Moreover, the presence of perforated sheets in the complicated GO membranes enables additional ion transport pathways that are not found in LK models. For ion transport studies, the free energy barriers for single-ion transport indicated significant differences based on the chemistry of the hole edges, the hole size and the ion type.

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