



THE UNIVERSITY OF
SYDNEY
—
Nano Institute

Network 4 Sustainable Nanotechnology Global Summit 2023

Affordable and clean energy
27 – 29 November 2023

The University of Sydney Nano Institute



WELCOME

Acknowledgement of Country

We recognise and pay respect to the Elders and communities – past, present, and emerging – of the lands that the University of Sydney's campuses stand on. For tens of thousands of years, they have shared and exchanged knowledges across innumerable generations for the benefit of all.

Welcome from the N4SN Global Summit 2023 Organising Committee

It is our great pleasure to bring together so many members of the Network for Sustainable Nanotechnology in person this November. This summit, our third in an ongoing series of N4SN meetings, is centred around one of the key challenges of our time – how to ensure a just transition to clean and affordable energy for all. We look forward to hearing about the technical and scientific progress within our community and to sharing our knowledge and understanding of the role of nanotechnology in achieving SDG7.

It has been our great pleasure to put together this program which celebrates multidisciplinary and collaboration and will allow time and space for important conversations between our community and the public.

Thank you so much for joining us: together we are delighted to welcome you to Sydney and hope you enjoy the summit!

Associate Professor Girish Lakhwani

Associate Professor Alice Motion

Associate Professor Yixiang Gan



Girish Lakhwani

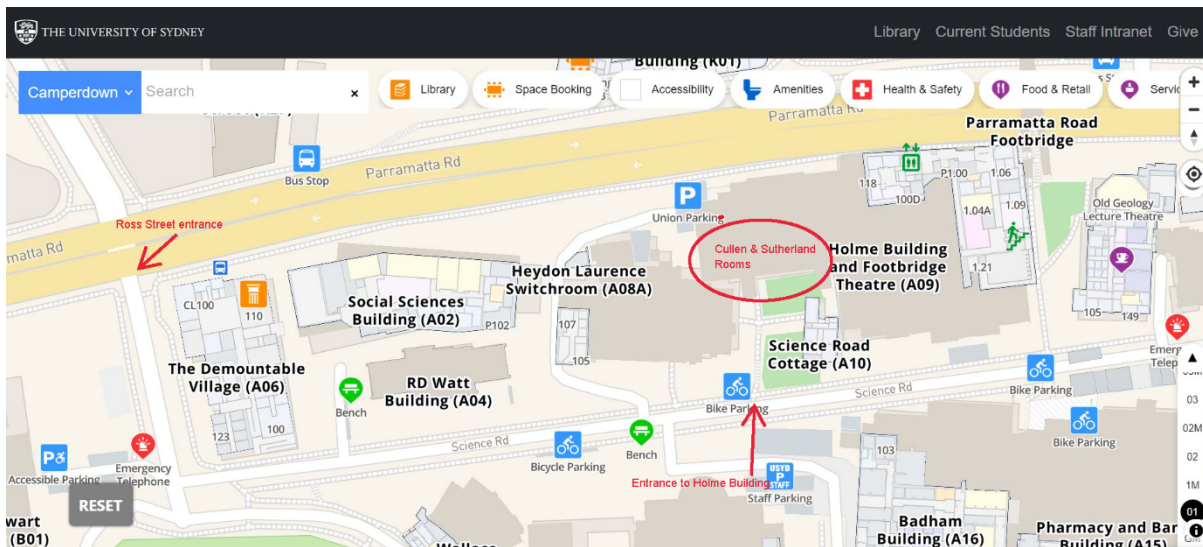
Alice Motion

Yixiang Gan

EVENT INFORMATION

Venue – Cullen Room, Holme Building (Building A09), Science Road, The University of Sydney

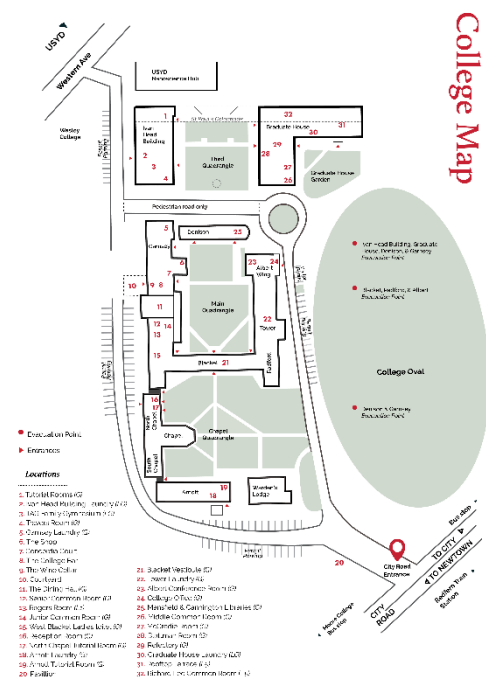
The Holme Building (A09) is set on The University of Sydney’s main campus of Camperdown. The Camperdown campus is situated less than 4 kilometres from Sydney’s CBD, and is most accessible **by public transport, cycling, walking** and rideshare however there are also **paid parking** options for **drivers**. The closest bus stop is the University of Sydney Footbridge bus stop on Parramatta Road. The nearest entrance is Ross Street, off Parramatta Road. If driving we recommend the **Shepherd St Carpark** on the corner of Cleveland St and Shepherd St. From there, it is a 14-minute walk to the Holme Building, walking via City Road and then Eastern Avenue.



View the Camperdown Campus [map](#)

Conference Dinner – St Paul’s College, Junior Common Room, 9 City Road, Camperdown

The conference dinner will be held in the Junior Common Room (14) at St Paul’s College Monday, 27 November. Please use the pedestrian gate via the main entrance via 9 City Road, Camperdown. It is a 16 minute walk from the Holme Building (A09). Please visit [Google Maps](#) for directions.



Live from the Lab – Charles Perkins Auditorium, Opposite Charles Perkins Main Entrance
(Building D17)

Live from the Lab is a celebration of Australian research, arts and culture.

This year our theme is *Clean and Affordable Energy* and we will feature the following researcher/musician partners in conversation with A/Prof Alice Motion together with a close listening to the new music:

- [Chiara Kovac](#) with [Prof Susan Park](#)
- [Gloomie](#) with [Prof Francois Aguey-Zinsou](#)
- [Setwun](#) with [Prof Anita Ho-Baille](#)
- [Huck Hastings](#) with [A/Prof Girish Lakhwani](#)

This is a free public N4SN Global Summit live event. Join us from 5pm for pre-dinner drinks and nibbles by registering via [Eventbrite](#).



View the Camperdown Campus [map](#) for walking instructions.

GUEST WIFI INSTRUCTIONS, THE UNIVERSITY OF SYDNEY

WiFi usage: In order to access the The University of Sydney WiFi network during your time on campus, you will need to follow these instructions:



Step 1. 'View wireless connection' and 'choose a wireless network' screen (see below for example).

Step 2. Select 'UniSydney-Guest'

Step 3. When you are successfully connected to 'UniSydney-Guest' click on your web browser ie safari, google, this will automatically take you to Sydney University page requesting the logon and password detail.

Please input the Username: **n4snsummit** and the password: **75469192** for the day a new screen will advise if you have succeeded in logging to the UniSydney-Guest network.

DISCLAIMER: Please note that we exercise no control over the nature, content or reliability of the information and/or data passing through our network

PLENARY SPEAKERS

Professor Rachel Caruso

Royal Melbourne Institute of Technology University



Professor Yun Liu

The Australian National University



KEYNOTE SPEAKERS

Professor Satish Patel

Indian Institute of Science



Professor Sally Brooker

University of Otago



INVITED SPEAKERS

Dr Kyra Schwarz

Deloitte Australia

Dr David Doral

Dovetail Electric Aviation

Dr Anastasia Globa

The University of Sydney

Prof Paul Dastoor

Newcastle University

Prof Anita Ho-Baillie

The University of Sydney

Prof Justin Hodgkiss

Victoria University of Wellington

A/Prof Yimin Yu

Waterloo Institute of Nanotechnology

Dr Shaikh Faisal

The University of Sydney

Dr Luke Liu

Victoria University of Wellington

Pradeep Murthy

The University of Sydney

A/Prof Luiz Ricardez Sandoval

Waterloo Institute of Nanotechnology

A/Prof Asaph Widmer-Cooper

Waterloo Institute of Nanotechnology

Prof Aaron Marshall

University of Canterbury

Dr Chang Wu

University of Canterbury

Prof Somnath Chanda Roy

Indian Institute of Technology

Mr Thomas Gao

NSW Decarbonisation Innovation Hub, UNSW

Prof Raghuram Chetty

Indian Institute of Technology (IIT) Chennai, India

Prof Chiara Neto

The University of Sydney

A/Prof Franck Natali

Victoria University of Wellington

Dr Francois Allieux

The University of Sydney

Prof Kondo-Francois Aguey-Zinsou

The University of Sydney

Prof Antonio Tricoli

The University of Sydney

Dr Yaning Wei

The University of Sydney

Dr Junma Tang

The University of Sydney

Dr Shubra Singh

Anna University



PANEL MEMBERS

Stephanie Bashir

Founder and CEO of Nexa Advisory, Board Member of the Smart Energy Council

Debbie Chen

Client Manager, Business Development at Australian Renewable Energy Agency (ARENA)

Professor Jaime Miranda

Professor and Head of School, Sydney School of Public Health, Faculty of Medicine, and Health

Professor Paul S. Weiss

Director of the California NanoSystems Institute, Professor of Chemistry and Biochemistry at UCLA, and Fred Kavli Chair in NanoSystems Sciences

Timothy Lang

NSW Organiser, Labor Environment Action Network

2023 N4SN Global Summit UNSDG 7: Affordable and Clean Energy

- Talk duration: Plenary - 35 mins, Keynote - 25 mins, Invited - 15 mins.
- Each talk will follow up with 5 min Q&A.
- Each session involves a 10-minute wrap-up discussion involving all session speakers.

Monday 27th Nov, Holme Building (A09), Cullen Room

8:30 – 9:15	Registrations and coffee reception
9:15 – 10:00	Welcome to Country Ceremony
10:00 – 10:20	Opening remarks

10:20 – 12:10	Session 1: Energy Applications and Australian context Chair: A/Prof Alice Motion, The University of Sydney
Plenary	Prof Rachel Caruso, RMIT, Melbourne, Australia "Varying the Composition and Morphology of Materials for Energy Applications"
Invited	Dr David Doral, Dovetail Electric Aviation "Electric Aviation and practical applications of battery and fuel cell technologies"
Invited	Dr Kyra Schwarz, Deloitte Australia "Key Trends in Sustainability and the Energy Transition 2023"
Invited	Mr Thomas Gao, NSW Decarbonisation Innovation Hub, UNSW "Navigating the NSW Clean Economy: Insights from the 2023 Decarbonisation Innovation Study"
Discussion/perspectives (10 mins)	

12:10 – 13:00	Lunch
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13:00 – 14:40	Session 2: Energy Harvesting, I (Photovoltaics) Chair: A/Prof Girish Lakhwani, The University of Sydney
Keynote	Prof Satish Patil, Indian Institute of Science, Bengaluru, India "Emerging Renewable Energy Technologies to Enable Net-Zero"
Invited	Prof Paul Dastoor, Newcastle University, Australia "Aqueous Dispersions of Organic Nanoparticles: Green Manufacturing of Printed Solar Cells"
Invited	Prof Justin Hodgkiss, Victoria University of Wellington, New Zealand "The Emergence of Non-fullerene Electron Acceptors for Efficient Printable Solar Photovoltaic Cells"
Invited	A/Prof Asaph Widmer-Cooper, The University of Sydney, Australia "Using Computer Simulations to help bring Perovskites Solar Cells to Market"
Discussion/perspectives (10 mins)	

14:40 – 15:00	Tea/coffee
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15:00 – 16:30	Session 3: Energy harvesting (cont.) and Storage I Chair: Prof Deanna D'Alessandro, The University of Sydney
Invited	Prof Anita Ho-Baillie, The University of Sydney, Australia "Multi-junction concepts for high performance solar cells"
Invited	Dr Shaikh Faisal, The University of Sydney, Australia "Highly Dispersible Nanocarbons for Energy Storage Applications"
Invited	Dr Luke Liu, Victoria University of Wellington, New Zealand "A High-Valent Organic Linker-Based Metal-Organic Framework for Selective Methane Capture"
Invited	Mr Pradeep Murthy, The University of Sydney, Australia "Nanocatalyst development and improvement for CO ₂ conversion"
Discussion/perspectives (10 mins)	

16:45 – 17:30	Sydney Nano Tour (Prof Simon Fleming, The University of Sydney)
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18:00 – 20:00	Summit Dinner, St Paul's College <i>For registrants who have RSVP'd.</i>
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Tuesday 28th Nov, Holme Building (A09), Cullen Room

8:30 – 9:15	Registration and coffee reception
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9:15 – 11:05	Session 4: Energy Harvesting II and management. Chair: Prof Justin Hodgkiss, Victoria University Wellington
Plenary	Prof Yun Liu, Australian National University, Australia "Nanostructural design for new bulk photovoltaic materials beyond conventional ferroelectricity"
Invited	Dr Junma Tang, The University of Sydney, Australia "Dynamic configurations of metallic atoms in the liquid state for selective propylene synthesis"
Invited	Elyas Asadi Shamsabadi, The University of Sydney, Australia "City Meta Twins Building Resilience"
Invited	Prof Raghuram Chetty, Indian Institute of Technology (IIT) Chennai, India "Performance of Electrodeposited Pt/Ti Catalyst Towards Methanol Oxidation Reaction"
Discussion/perspectives (10 mins)	

11:05 – 11:25	Tea/coffee
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11:25 – 12:35	Session 5: Energy Storage II Chair: Prof Kondo-Francois Aguey-Zinsou, The University of Sydney
Invited	Prof Aaron Marshall, University of Canterbury, New Zealand "Understanding and improving the activity of carbon felt electrodes for redox flow batteries"
Invited	Dr Chang Wu, University of Canterbury, New Zealand "Achieving high current density performance of OER with NiFeMn LDH"
Invited	Prof Somnath Chanda Roy, Indian Institute of Technology, Chennai "Addressing the competing adsorption bottleneck in photocatalytic CO ₂ reduction by using hydrophilic-hydrophobic heterojunctions : a novel pathway to enhance product yield"
Discussion/perspectives (10 mins)	

12:35 – 13:30	Lunch
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13:30 – 15:10	Session 6: Energy Sustainability I Chair & Discussant: A/Prof Yixiang Gan, The University of Sydney
Keynote	Prof Sally Brooker, Otago University, New Zealand He Honoka Hauwai / German-New Zealand Green Hydrogen Centre for Research, Networking and Outreach
Invited	Prof Chiara Neto, The University of Sydney, Australia "Advanced Capture of Water from the Atmosphere Using Daytime Radiative Passive Cooling"
Invited	A/Prof Franck Natali, Victoria University of Wellington, New Zealand "Energy-Efficient Catalysts For Green Ammonia Synthesis"
Invited	Dr Francois Allieux, The University of Sydney, Australia "Catalytic high-entropy low melting point metal nanodroplets"
Discussion/perspectives (10 mins)	

15:10 – 15:30	Tea/coffee
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15:30 – 17:00	Session 7: Energy production and sustainability II Chair & Discussant: A/Prof Yixiang Gan, The University of Sydney
Invited	Prof Kondo-Francois Aguey-Zinsou, The University of Sydney "Materials for the Hydrogen economy"
Invited	Prof Antonio Tricoli, The University of Sydney, Australia "Design of Scalable Nanoscale Electrocatalysts for Green Hydrogen and E-Fuels Production"
Invited	Dr Yaning Wei, The University of Sydney, Australia "Addressing Environmental Sustainability in Wind Energy: Recycling Composite Materials in Wind Turbine Blades"

Invited	Dr Shubra Singh, Anna University, Chennai, India "Design and development of nanomaterials for removal of emerging categories of persistent organic pollutants in contaminated water"
Discussion/perspectives (10 mins)	

17:00 – 19:30	Live from the Lab (LFTL) event, Charles Perkins Centre Auditorium LFTL is a celebration of Australian research, science, arts and culture. Since 2020, LFTL has united science researchers with musicians through a guided conversation series and commission new musical responses to ground-breaking Australian research. This year the LFTL theme is "SDG7 Affordable and Clean Energy" Register here	
	Refreshments will be served from 5pm and the event will run 6 - 7:30pm.	
	Academics	Artists
	Prof Susan Park	Chiara Kovac
	Prof Francois Aguey-Zinsou	Gloomie
	Prof Anita Ho-Baille	Setwun
	A/Prof Girish Lakhwani	Huck Hastings

Wednesday 29th Nov, Holme Building (A09), Cullen Room

8:30 – 9:30	Registrations, welcome and coffee
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9:30 – 11:30	Session 8: Panel Discussion
Panel Discussion	<p>"How to achieve public policy progress in the clean energy sector"</p> <p>Moderator: A/Prof Alice Motion, The University of Sydney</p> <p>Panellists:</p> <ul style="list-style-type: none"> • Stephanie Bashir Founder and CEO of Nexa Advisory, Board Member of the Smart Energy Council • Deb Chen Client Manager, Business Development at Australian Renewable Energy Agency (ARENA) • Professor Jaime Miranda Professor and Head of School, Sydney School of Public Health, Faculty of Medicine, and Health • Professor Paul S. Weiss Director of the California NanoSystems Institute, Professor of Chemistry and Biochemistry at UCLA, and Fred Kavli Chair in NanoSystems Sciences • Timothy Lang NSW Organiser, Labor Environment Action Network

11:45 – 13:00	Break-out sessions on Australia & UNSDG7 with lunch
13:00 – 13:45	Feedback session
13:45 – 14:00	Prize ceremony and summit close

COMMITTEE

Special thanks go to our conference organising and scientific committee members and session chairs:

- **A/Prof Girish Lakhwani** (Organising Committee, co-Chair) The University of Sydney
- **A/Prof Alice Motion** (Organising Committee, co-Chair) – The University of Sydney
- **A/Prof Yixiang Gan** (Organising Committee) The University of Sydney
- **Prof Deanna D'Alessandro** (Scientific Committee and Session Chair) The University of Sydney
- **Prof Justin Hodgkiss** (Scientific Committee and Session Chair) Victoria University Wellington
- **A/Prof Yimin Yu** (Scientific Committee and Session Chair) Waterloo Institute of Nanotechnology
- **Prof Kondo-Francois Aguey-Zinsou** (Session Chair) The University of Sydney
- **Prof Nicola Gaston** (Session Chair) The University of Auckland



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Varying the Composition and Morphology of Materials for Energy Applications

Haoxin Mai,¹ Xuying Li,¹ S. Amanda Ekanayake,¹ Dilek Korcoban,¹ Tu Le,² Dehong Chen,¹ David A. Winkler³ and Rachel A. Caruso^{1*}

¹ RMIT University, ² RMIT University, ³ Monash University

¹ Applied Chemistry and Environmental Science, School of Science, RMIT University, Victoria, Australia;

² School of Engineering, RMIT University, Victoria, Australia; ³ Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Victoria, Australia

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Decreasing greenhouse gas emissions and reaching “net zero” has become a common mantra for companies, states and countries around the globe. Given the large contribution the production and use of energy has to these emissions, there has been an increasing research focus on materials and technologies for clean energy generation and storage, along with emission capture, storage or conversion.

My research group has investigated the effect of the materials morphology,¹ the addition of a dopant² and the formation of heterostructures on the properties of materials that have potential application in solar cells, batteries and as photocatalysts for fuel production (e.g., H₂)³ and pollutant degradation.⁴ By manipulating the structure, porosity, surface area or composition using a range of chemical synthesis approaches, the performance of these materials can be improved. Synthesis using hydrothermal/solvothermal treatment, hot injection methods, self-assembly or preformed templates, can be used to vary these parameters. When there is a large variety of possible compositions, such as for perovskites, machine learning techniques have also been employed to aid in the discovery and design of materials.^{3,5}

In this presentation, examples will be given that demonstrate a number of these approaches for varying the composition and morphology of materials, with a focus on materials that can be applied in the areas of energy conversion and storage.

This research was supported by ARC Discovery Projects (DP180103815 and DP220100945).

References

1. H. Mai, X. Li, J. Lu, X. Wen, T. C. Le, S. P. Russo, D. Chen, R. A. Caruso, *J. Am. Chem. Soc.* **2023**, 145, 17337.
2. X. Li, H. Mai, N. Cox, J. Lu, X. Wen, D. Chen, R. A. Caruso, *Chem. Mater.* **2023**, 35, 3105.
3. H. Mai, T. C. Le, T. Hisatomi, D. Chen, K. Domen, D. A. Winkler, R. A. Caruso, *iScience* **2021**, 24, 103068.
4. H. Mai, D. Chen, Y. Tachibana, H. Suzuki, R. Abe, R. A. Caruso, *Chem. Soc. Rev.* **2021**, 50, 13692.
5. H. Mai, T. C. Le, D. Chen, D. A. Winkler, R. A. Caruso, *Chem. Rev.* **2022**, 122, 13478.



N4SNano Global Summit 2023
The University of Sydney nano Institute, 27-29 November 2023

Key Trends in Sustainability and the Energy Transition 2023

Kyra N Schwarz^{1*}

¹ *Deloitte Australia, VIC, Australia*

*Email: kyschwarz@deloitte.com.au

The energy transition refers to the global energy sector's shift from fossil-based systems of energy production and consumption. Meeting the global demand for energy while playing a meaningful role in emissions reductions is a balancing act that requires governments and organisations to act quickly and evolve in their thinking.

Australia is in the midst of an energy transformation with a variety of opportunities emerging across all sectors with innovation and technology continuing to play a critical role.

This talk will outline the current status of the energy transition, and the key trends shaping its outlook.



Microsoft Word Template for Abstracts for N4SNano Global Summit
Anastasia Globa 1*, Elyas Asadi Shamsabadi 2, Daniel Dias-da-Costa 2, Zihao Liu 2, Arianna Brambilla 1, and Luming Shen 2

¹ University of Sydney,

¹ School of Architecture, Design and Planning, the University of Sydney, NSW, Australia; ² School of Civil Engineering, Faculty of Engineering, the University of Sydney, NSW, Australia;

*Email: anastasia.globa@sydney.edu.au

City Meta Twins – Building Resilience

Climate-related disasters are becoming more frequent and imposing growing risks onto societies. Over the past decade, the damages associated with natural disasters have multiplied. With the world's ever-changing dynamics, our project aims to establish an interactive meta-twin hub where accurate digital replicates of the real-world merge with AI and remote sensing to virtually recreate first-hand disaster effects on infrastructure assets to significantly enhance proactive measures and mitigation strategies.

We focus on bushfires as a proof-of-concept aiming to improve Australia's resilience to bushfires. 'Build back better' is often used to support resilience against climate change and bushfires in human settlements, yet there remains a limited understanding of how we could enable the real-time collection, fusion, and processing of data from diverse sources to effectively unify humanitarian relief and disaster response and recovery actions; and how we can effectively engage with communities to raise awareness, educate and encourage safe practices locally.

The first stage of the project was conducted using parametric modelling and gaming engines to simulate the impacts of auxiliary structures in bushfire events ¹. Four simulation approaches were explored including Shortest Path, Heat Map, Vector field and Particle systems. The next research stage will explore the use of Unreal Engine to develop an immersive City Meta Twin - and test various bushfire scenarios. The study aims to implement the proof of concept to validate the viability of the meta-twin hub, and to establish collaboration with global emergency response organisations to refine our objectives and seize new opportunities.

Acknowledgements: *The authors would like to acknowledge the contribution of Dr Dagmar Reinhardt, Dr Adrienne Keane (USYD) and Dr Peter Davies (Macquarie University) – first stage prototype and approach development. The authors would also like to acknowledge Sydney Nano who generously supports this initiative through the Kickstarter Award (2023/2024)*

FIRE SPREAD PROBABILITY

PARTICLE SYSTEMS

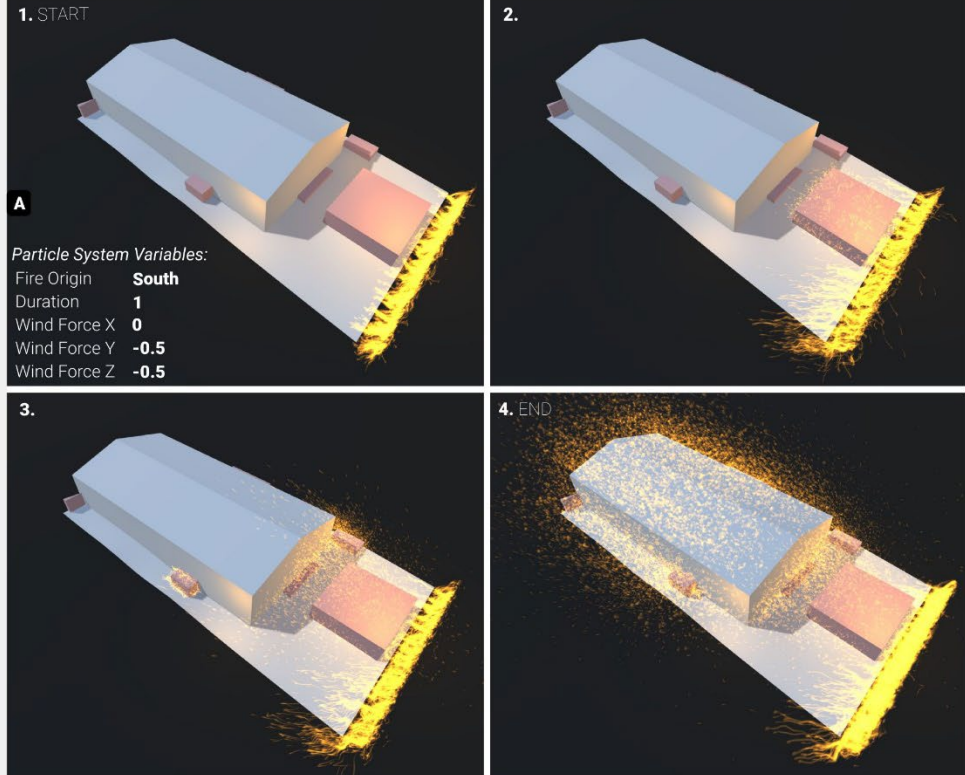
Simulation approach

Use the combination of physics engine, collisions and Particle systems in Unity 3D to simulate fire spread.

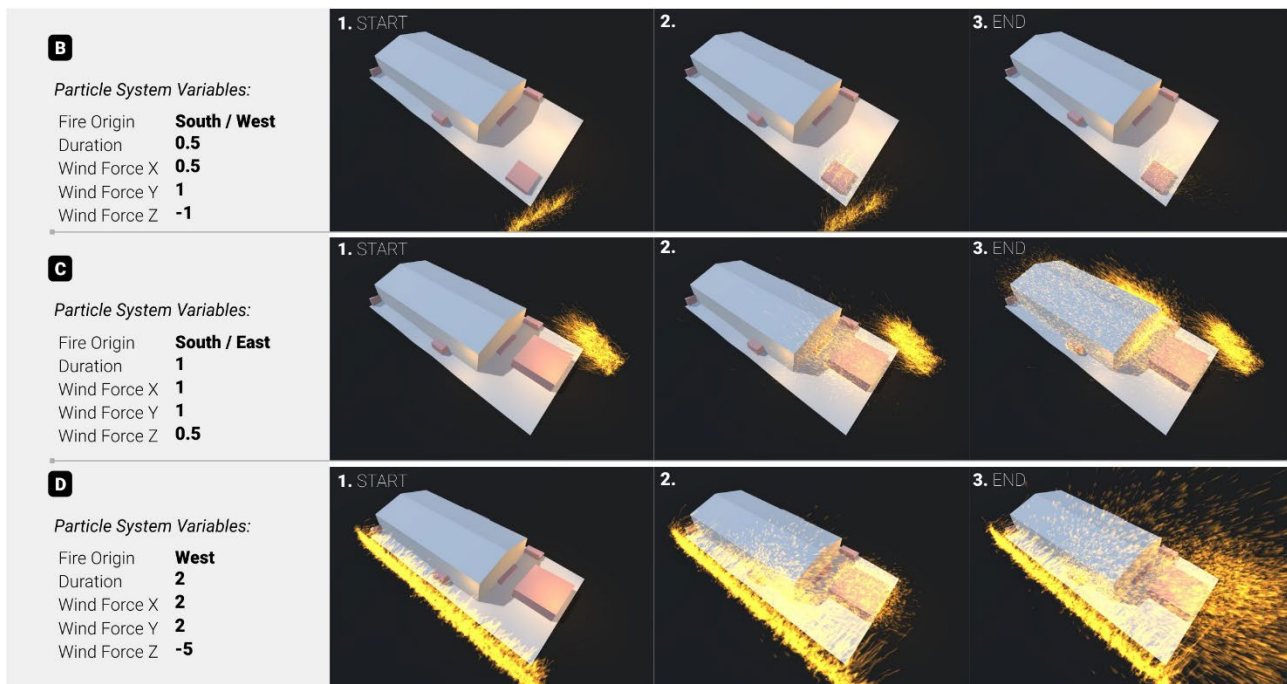
- 1) Choose location and size of initial fire source (setting a mesh object as the system 'shape' reference).
- 2) Control strength of fire with the number of emitted particles, their size and duration.
- 3) Use particle trails to show fire movement.
- 4) Set-up auxiliary structures as sub-emitters that are activated on collision. When the 'fire' particles hit auxiliary structure mesh.
- 5) Use 'Force over time' as a means of controlling wind strength and direction.

Colour-coding:

Particle colour overtime



Fire spread probability simulation: Particle Systems (Unity) - Method.



Fire spread probability simulation: Particle Systems (Unity) - Iterations.

FIRE SPREAD PROBABILITY

HEAT MAP

Simulation approach

1. Determine flammable and non-flammable elements in the system.
2. Calculating affected area based on the proximity to the flammable objects & visualising 'heat' map using a gradient: from 'high' to 'low' fire risk areas.

1	-2	+3	1	-1	+3
0	1	2	0	-1	+3
0	0	+3	0	1	0
1	1	+2	+1	0	+1
-2	-1	+1	0	0	0
0	-2	-1	1	-1	0

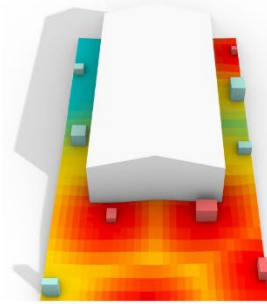
Simulation Variables:

- Ground Surface Subdivision **30x30**
- Elements Flammable (%) **50**
- Elements Non-flammable (%) **50**

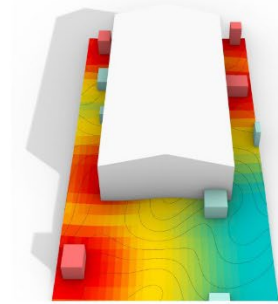
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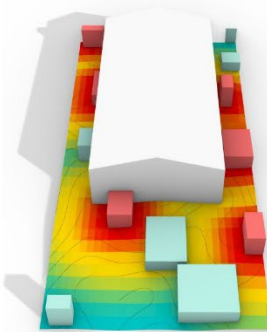
SS1



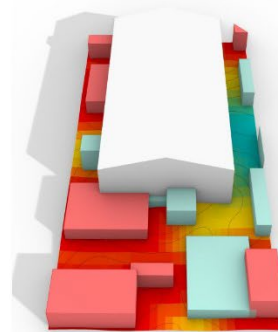
SS3



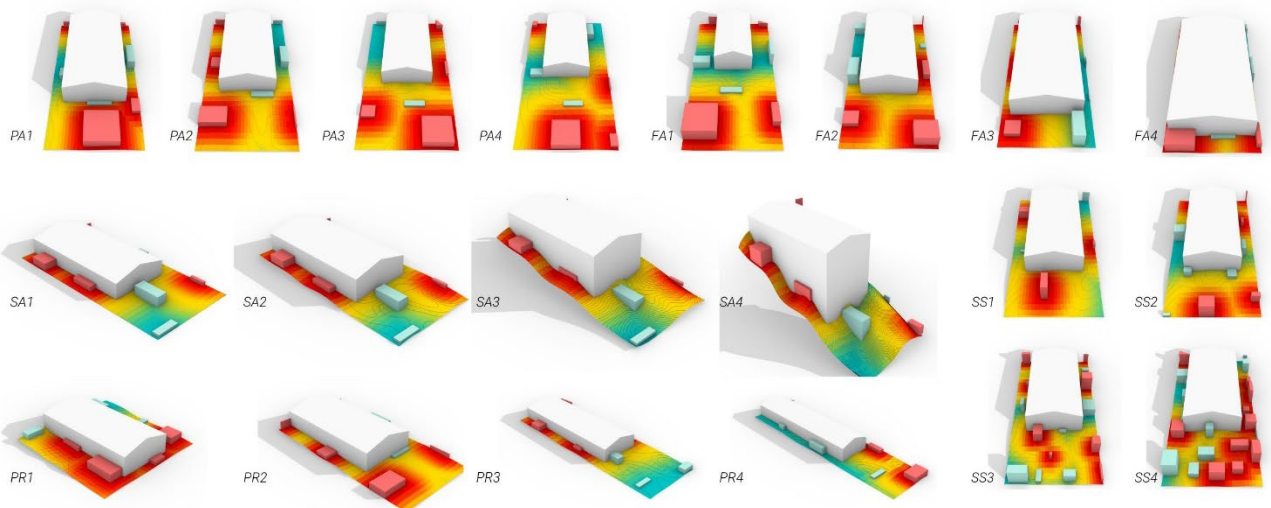
SS2



SS4



Fire spread probability simulation: Heat Map - Method.



Fire spread probability simulation: Heat Map - Iterations.

FIRE SPREAD PROBABILITY

VECTOR FIELD

Simulation approach

1. Create 'charge' vectors along the perimeter of flammable elements in the system and the closest points on the surface grid, with vectors pointing outwards to simulate emitting radiant heat and embers.

2. Simulate different wind forces varied across all three dimensions X, Y, Z.

3. Add two vector forces together for each location point and visualise resulting vector field.

Simulated for four force combination scenarios: A, B, C & D

Simulation Variables:

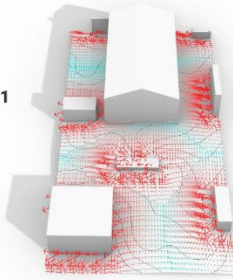
Ground Surface Subdivision **60x60**
Elements Flammable (%) **100**
Elements Non-flammable (%) **0**

Colour-coding:

High Fire Risk Low Fire Risk
Max **Min**

A
Vector Force Variables:
Elements Charge emitting power (m) **0.5-1**

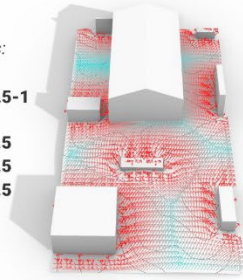
Wind Force X (m) **0**
Wind Force Y (m) **0**
Wind Force Z (m) **0.5**



FA1

B
Vector Force Variables:
Elements Charge emitting power (m) **0.5-1**

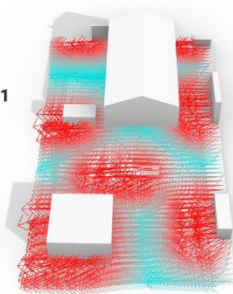
Wind Force X (m) **0.5**
Wind Force Y (m) **0.5**
Wind Force Z (m) **0.5**



FA1

C
Vector Force Variables:
Elements Charge emitting power (m) **0.5-1**

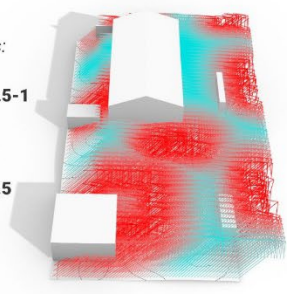
Wind Force X (m) **-2**
Wind Force Y (m) **-1**
Wind Force Z (m) **0.8**



FA1

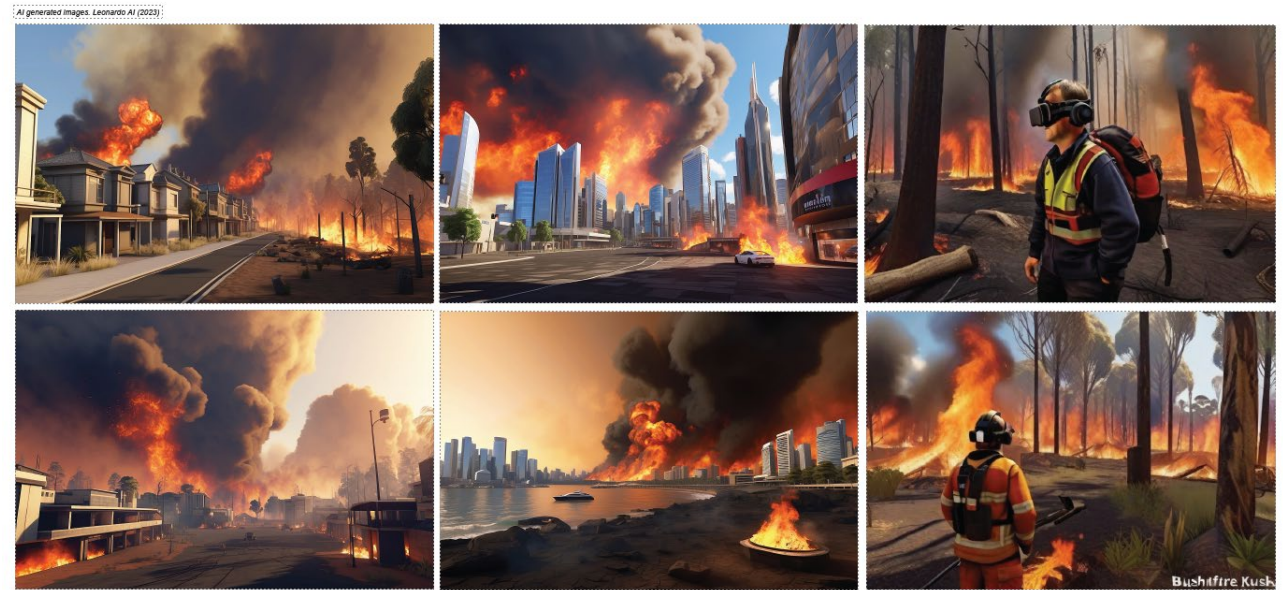
D
Vector Force Variables:
Elements Charge emitting power (m) **0.5-1**

Wind Force X (m) **4**
Wind Force Y (m) **3**
Wind Force Z (m) **1.5**



FA1

Fire spread probability simulation: Vector Field - Method.



AI-generated Vision based on meta city and bushfire prompts (Leonardo AI).

References:

¹ Globa, A., Reinhardt, D., Keane, A., & Davies, P. (2022). Building resilience: using parametric modelling and gaming engines to simulate the impacts of secondary structures in bushfire events. In *27th International Conference for The Association for Computer-Aided Architectural Design Research in Asia, CAADRIA 2022* (pp. 749-758). Association for Computer-Aided Architectural Design Research in Asia (CAADRIA).



Aqueous Dispersions of Organic Nanoparticles: Green Manufacturing of Printed Solar Cells

Paul Dastoor

University of Newcastle

¹ *Centre for Organic Electronics, University of Newcastle, NSW, Australia*

* Email: Paul.Dastoor@newcastle.edu.au

Aqueous Dispersions of Organic Nanoparticles: Green Manufacturing of Printed Solar Cells.

Printed solar modules based on organic photovoltaic materials offer significant promise as a next-generation solar energy technology manufactured using roll-to-roll printing. Printed solar weighs less than 300 g per square metre, is less than 0.3 mm thick and can be adhered to roofing using adhesives. Detailed economic modelling has demonstrated that by focussing on low-cost materials and manufacturing techniques, printed solar is commercially compelling at lower device efficiencies and lifetimes than conventional solar panels [1].

A key application is the Industrial, Warehouse and Commercial (IWC) building sector, conservatively estimated to be over 100 million sqm in Australia [2] and over 4 billion sqm worldwide [3]. IWC roofs are manufactured to the minimum specification and incapable of supporting the weight of conventional silicon solar panels.

Water-based organic nanoparticle dispersions (solar paint) provide a route to completely green manufacturing of printed solar cells. The nanoparticle approach offers a new generation of inexpensive nanomaterials produced at commercial scale under eco-friendly conditions. However, the structure-function of these nano-colloidal systems is complex and requires characterisation techniques that can map chemical structure in three dimensions on the nanoscale. This paper will describe the structure-function relationships of organic electronic nanoparticulate thin films used in organic photovoltaics, from small scale devices all the way up to large scale printed solar cells. In particular, the role that synchrotron X-ray techniques can play in characterising these materials will be discussed. Finally, the future prospects and economics for large scale manufacture of solar cells based on printing will be explored.

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The emergence of non-fullerene electron acceptors for efficient printable solar photovoltaic cells

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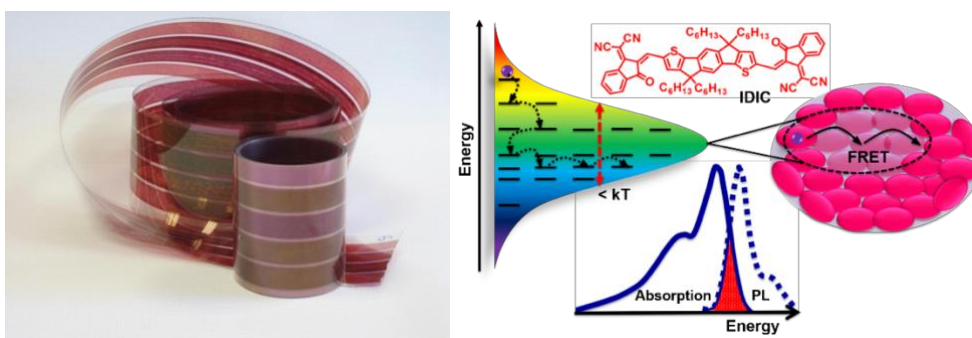
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Organic carbon-based semiconductors offer immense promise for photovoltaic applications because of their strong optical absorption, chemically tuneable optoelectronic properties, and their compatibility with simple manufacturing processes like printing.¹

The strong binding between charge pairs, or exciton binding, in organic photovoltaic (OPV) cells requires junctions between donor and acceptor materials to separate charges. Whereas donor materials evolved considerably, acceptor materials were, until recently, constrained to carbon fullerenes, in spite of their poor optical absorption and chemical tuneability.

In this talk, I will describe the emergence and remarkable properties of non-fullerene acceptors, focusing on the discovery and implications of rapid and long-range exciton diffusion. Modest exciton diffusion lengths dictate the need for nanostructured bulk heterojunctions in OPV cells, however, this morphology compromises charge collection. Here, we reveal rapid exciton diffusion in films of high performing fused-ring non-fullerene acceptors. Using experimental² and computational³ approaches, rapid exciton diffusion is shown to arise from intrinsic molecular and packing factors and can even now be screened computationally. Relieving exciton diffusion constraints has important implications for OPVs; large, ordered, and pure domains – even bilayer architectures⁴ – enhance charge separation and transport, and suppress recombination, thereby boosting fill factors and efficiencies.



Printed OPV cell (left), exciton diffusion in the non-fullerene acceptor, IDIC (right)

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Cascade electrocatalysis via AgCu single atom alloy and Ag nanoparticles in CO₂ electroreduction towards multicarbon products

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Development of sustainable and clean sources of energy, and mitigation of greenhouse gas emissions such as CO₂, is among the greatest challenges facing our planet. Electrocatalytic CO₂ reduction into value-added multicarbon products offers a means to close the anthropogenic carbon cycle using renewable electricity. However, the unsatisfactory catalytic selectivity for multicarbon products severely hinders the practical application of this technology. We report a cascade AgCu single-atom and nanoparticle electrocatalyst, in which Ag nanoparticles produce CO and AgCu single-atom alloys promote C-C coupling kinetics. As a result, a Faradaic efficiency (FE) of $94 \pm 4\%$ toward multicarbon products is achieved with the as-prepared AgCu single-atom and nanoparticle catalyst under $\sim 720 \text{ mA cm}^{-2}$ working current density at -0.65V in a flow cell with alkaline electrolyte. Density functional theory calculations further demonstrate that the high multicarbon product selectivity results from cooperation between AgCu single-atom alloys and Ag nanoparticles, wherein the Ag single-atom doping of Cu nanoparticles increases the adsorption energy of *CO on Cu sites due to the asymmetric bonding of the Cu atom to the adjacent Ag atom with a compressive strain.

Microsoft Word Template for Abstracts for N4SNano Global Summit Shaikh Nayeem Faisal

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Highly Dispersible Nanocarbons for Energy Storage Applications

Abstract: Nanostructured materials are playing crucial role in renewable energy engineering by improving the electro-catalytical properties for green hydrogen production via water splitting, the capacitance in lithium-ion batteries as well as future energy system as photo-chargers, thermo-cells and thermal energy storage. The recently invented highly dispersible edge-functional graphene has been demonstrated as a key element for shapable supercapacitors, developing high performance anode in lithium-ion batteries (commercialized by Sicona Battery Technology Pty Ltd.),¹ wearable thermocells,² and flexible printed photo-chargers. In this presentation, I am going to present my work on nanocarbon and graphene for next generation energy storage system.

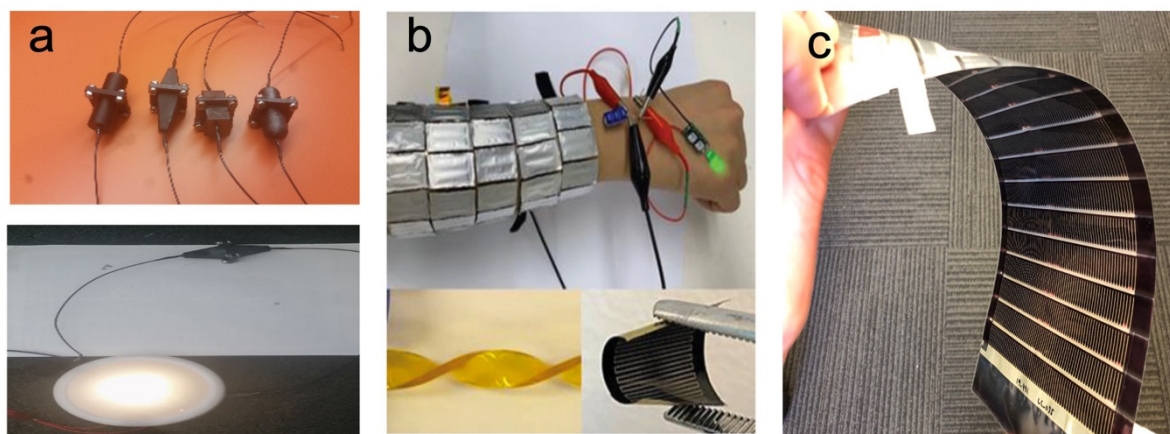


Figure 1. a) shapable supercapacitors, b) wearable thermocells to produce electricity from body heat, c) flexible printed photo-chargers.

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A High-Valent Organic Linker-Based Metal-Organic Framework for Selective Methane Capture

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Methane is a potent greenhouse gas contributing to around 30% global warming.¹ While flaring has been implemented in energy sector to convert methane into CO₂ – a much less potent greenhouse gas, mitigating emissions from sources where methane concentration is low, remains a major challenge. As such, materials that can selectively adsorb methane are highly desirable.

Although research into selective methane capture is in its infancy, characteristics for optimal methane storage materials are well understood. Large-scale screening of over 137,000 hypothetical metal-organic frameworks (MOFs) suggests that the most frequent pore sizes among the top-performing materials are 4 and 8 Å, just big enough to fit one or two methane molecules.² However, most of these top-performers pillar-layered structures are synthetically challenging due to their tendency to interpenetrate and deform upon solvent removal.

To tackle this synthetic challenge, we designed a high-valent organic linker with geometry resembling a metal cluster used in MOFs. This unique linker produced a MOF with optimal structure characteristics for methane capture. Our preliminary data suggests that this material has a striking CH₄/N₂ selectivity over 10 and is among the two most selective methane adsorbents reported.

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Nanocatalyst development and improvement for CO₂ conversion

Global warming poses many environmentally damaging effects, and the most predominant contributor is carbon dioxide (CO₂), which is generally produced from excessive fossil fuel consumption.¹ The need to mitigate atmospheric CO₂ levels is therefore imperative.

The quickest and most efficient remedy is to capture and convert CO₂ directly into valuable, low-emission fuels, such as carbon monoxide (CO) and methane (CH₄) for mining, transport or domestic applications, by reacting it over a catalyst, which at nanoscale will have more surface area over which to catalyse CO₂ reduction.^{2,3}

The most effective catalytic reaction to convert CO₂ is hydrogenation, as hydrogen (H₂), which can be obtained greenly via electrolysis, can easily react with the CO₂ molecule at elevated temperatures.⁴ Our research involves a very effective and selective catalyst containing nanoparticles of ruthenium (Ru), a highly active metal that can effectively adsorb H₂,^{5,6} embedded over a nitrogen-doped carbon nanosphere (N-CNS) support,⁷ a structurally stable material and which can both bind CO₂ and keep the ruthenium nanoparticles in place.² Such a combination has enabled greater CO₂-H₂ interaction and conversion to generate the valuable products.

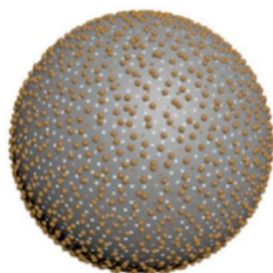


Figure 1. An example Ru/N-CNS catalyst. Image taken from Liu et al.²

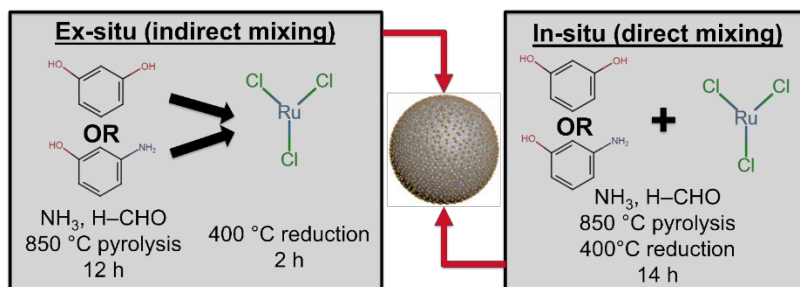


Figure 2. Synthesis methods used to form the Ru/N-CNS catalysts. The image of the Ru/N-CNS material was taken from Liu et al.²

Our key findings, through laboratory, computational, and economic analyses, are that Ru/N-CNS, when synthesised with 3-aminophenol and by an *in-situ* (i.e., direct mixing) method, has a strong bifunctional effect between Ru and N-CNS to reach 60% CO₂ conversion and 95% CO selectivity and can generate a profitable 0.36 USD kg⁻¹ CO (currently 0.55 USD kg⁻¹).⁸ Thus, such a material has foreseeable commercial application towards reaching a greener future.

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Nanostructural design for new bulk photovoltaic materials beyond conventional ferroelectricity

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Photovoltaic (PV) is a process converting light energy to electrical energy. A highly efficient PV effect relies on two factors: (i) a high photocurrent and (ii) a built-in electric field enabling the separation of the photogenerated electrons and holes. In traditional PV devices, electron-hole pairs are generated by light absorption in narrow bandgap semiconductors, and then separated through the depletion field in the heterojunction. The maximum voltage of these devices, however, equals to their bandgap, and thus the power conversion efficiency is restricted by Shockley–Queisser limitation. To break this limitation and obtain higher voltage, ferroelectric (FE) materials, due to their non-centrosymmetric structures that can induce stable depolarization electric fields and generate much higher photovoltage than their bandgap (named as bulk PV effect), have received a renewed attention in the PV application. Despite the high voltage the FE materials can exhibit, the photocurrent of most of the FE materials is really low because of their wide bandgaps resulting in the low conductivity and the deficient absorption of the solar energy. In this talk, we will present a new strategy to create bulk PV effect though structurally or chemically restructuring narrow bandgap, non-ferroelectric metal oxide semiconductors, in which high performance ferroelectric properties are achieved without significantly changing their intrinsic electronic and photoelectronic properties. It is found that in such a way, the modified materials show a ferroelectric like bulk photovoltaic effect and enhanced photocurrent (10^3 – 10^4 times higher than that of conventional ferroelectric materials and comparable to state-of-the-art multilayered multiferroics). Such a new type of bulk photovoltaic materials lightens a potential for practical use in solar energy conversion.



A Machine Learning-DFT Framework to Accelerate the Discovery of Catalyst Materials: An application of Catalyst Design for CO₂ Utilization

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This study presents a computational framework aimed to accelerate the discovery of novel catalyst materials for various applications, e.g., CO₂ utilization. The catalyst materials proposed by the framework are obtained from a machine learning (ML) framework that only requires a limited amount of data for training, which is the typical condition found in an actual setting. The framework makes use of First-principles Density Functional Theory (DFT) calculations to predict adsorption and activation energies for a different set of testing materials. Due to high computational costs, only a limited amount of DFT calculations can be obtained in acceptable turnaround times. Hence, the limited DFT results are used to train the proposed ML method, i.e., fine-tune a pre-trained neural predictor that approximates DFT predictions for adsorption and activation energies. Meta-learning and domain adaptation techniques are used to adapt the predictor specifically for the discovery of promising catalyst materials within a Bayesian optimization framework. Experimental testing has been conducted to support the theoretical DFT calculations and therefore the predictions from the proposed ML framework. To illustrate the benefits of the proposed computational framework, a case study involving the discovery of effective and energy efficient M-Ceria catalyst materials for CO₂ hydrogenation via the reverse water shift reaction is considered. Results show that the identified novel M-Ceria catalysts can effectively enhance product yield and selectivity to transform CO₂ into CO thus demonstrating the potential of this framework not only to transform CO₂ into valuable chemicals but to address computer-aided materials design for other major applications.



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Using Computer Simulations to help bring Perovskites Solar Cells to Market.

One of the key materials challenges in meeting UN Sustainable Development Goal 7 on Affordable and Clean Energy is to increase the efficiency of solar cells while making them cheaper, less energy-intensive and faster to manufacture. Metal halide perovskites are a promising class of semiconducting materials for achieving these goals, due to their ability to be solution processed near ambient conditions, the ease with which their bandgap can be tuned, and their tolerance to defects.¹ While solar cells with impressively high efficiencies have now been made using metal halide perovskites, their usefulness has been limited by poor materials stability to moisture and light. Another important challenge in bringing perovskite solar cells to market is to scale up the manufacture of high-quality crystalline films, which in turn requires detailed understanding of how these ionic crystals form starting from their solvated precursors.

In this talk, I will discuss some of the computational approaches that we have developed to tackle these problems and the insights we have gained from this work. This includes the development of models for studying the complex effects of light and heat on the bandgap of mixed halide perovskites² and for studying the formation of MHPs from solution,^{3,4,5}

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Understanding and improving the activity of carbon felt electrodes for redox flow batteries

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Redox flow batteries are a promising technology for providing large scale energy storage and the performance improvements from modifying the carbon felt electrodes has been studied in depth. Despite the wealth of research, decoupling the different effects (mass transport, surface area, wettability and kinetics) that ultimately contribute to overall battery performance is very complex. For example, the most common method (cyclic voltammetry) to determine the inherent kinetics of redox reactions is problematic due to the complex mass transport behaviour within these electrodes¹. By either avoiding or accounting for these complexities more accurate determination of kinetic information can be obtained, while also providing insights into spatial variation within carbon felt materials²⁻⁵. Similarly, understanding how the reaction kinetics are influenced by the presence oxygen- or nitrogen-functional groups, is extremely challenging as the kinetic effects can also be due to defects and edge sites which also facilitate the redox reactions^{6,7}. Unfortunately, it is hard to independently control only the content functional groups, as most O- or N-doping methods often cause unintentional changes in the carbon structure. Recently to investigate these issues, we have introduced catalytic sites into carbon and graphite felts using ion beam implantation. By using both N_2^+ - and Ne^+ -ion implantation it is possible to separate out the effects of nitrogen content vs defects and edges sites. While this method provides fundamental insights in catalytic activity, it also reveals that the fraction of carbon felt which is involved in the electrochemical processes may be quite low, suggesting that optimising the location catalytic sites may have some benefits.

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The increasing demand for hydrogen has brought academic eye into Anion Exchange Membrane Water Electrolyser (AEMWE), an attractive emerging green hydrogen technology. However, the sluggish anodic reaction (Oxygen Evolution Reaction) seriously hinders AEMWE device efficiency. Thus, the design of high-efficiency, low cost OER catalyst is critical. Transition metal layer double hydroxide has been proved to be a promising candidate to replace the noble metal catalyst. In this work, a series of nickel-based layer double hydroxide (LDH) has been electro-deposited on nickel foam as high- efficiency oxygen evolution reaction (OER). As a result, the NiFe_{0.75}Mn_{0.25} LDH exhibited the best electrochemical performance of overpotentials of 600 mV at extremely high current density of 2 A cm⁻² with 300 hours. Consequently, the boosting of electrochemical performance can be contributed to the tuning of Fe and Mn elements in Ni-based LDH, which modules the electronic contribution and Ni- O bond length. Furthermore, this LDH can be applied into AEMWE for exploring the industrialization of hydrogen production via water splitting.



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Addressing the competing adsorption bottleneck in photocatalytic CO₂ reduction by using hydrophilic-hydrophobic heterojunctions : a novel pathway to enhance product yield

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Solar powered conversion / reduction of carbon dioxide into value added chemicals has been identified as one of the foremost challenges for materials science in the 21st century. Despite extensive research, product yield remained low and one of the primary factors has been the issue of competing adsorption of CO₂ and water vapour on the catalyst surface. In this work we employ reduced graphene oxide wrapped TiO₂ nanotubes (TiO₂ - rGO) as a heterojunction photocatalyst and demonstrate that UV irradiation induces hydrophilicity on the TiO₂ surface and, hydrophobicity on the rGO surface. The resulting photocatalyst shows 25% higher yield of methane over that of untreated photocatalyst. Hence, UV irradiation induced tailoring of the hydrophilicity yields selective adsorption sites for the CO₂ and water vapour leading to a significant enhancement of the methane yield through photocatalytic reduction process.

He Honoka Hauwai / German-New Zealand Green Hydrogen Centre for Research, Networking and Outreach

Sally Brooker^{*,1} and Paul Jerabek²

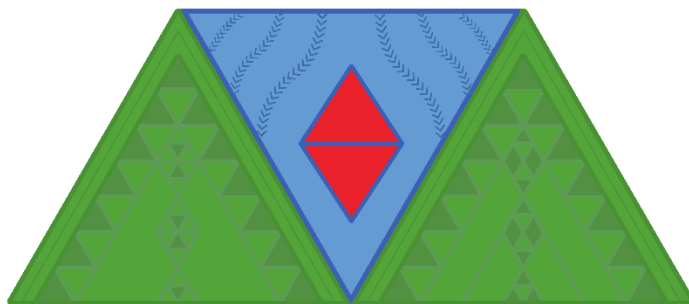
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Climate change requires rapid replacement of our present range of carbon-emitting fossil fuels (coal, oil, natural gas) by a suite of carbon-zero and carbon-neutral fuels. The best carbon-zero fuel is direct electrification (from renewable generation), followed by batteries and green hydrogen.

And overview of the place of green hydrogen as a key industry chemical, as well as in the suite of future fuels, when be presented, followed by an introduction to He Honoka Hauwai and our German-NZ-wide team's activities.



He Honoka Hauwai
German-NZ Green Hydrogen Centre

*He honoka hauwai,
he hirikapo auaha
A hydrogen alliance,
uniting innovative minds*

Acknowledgement: We are grateful to the BMBF (Germany) and MBIE (New Zealand) for jointly funding 4 grants, supporting the establishment of this alliance as well as three research projects.



Advanced Capture of Water from the Atmosphere Using Daytime Radiative Passive Cooling

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Atmospheric water capture has the potential to alleviate water scarcity around the world by condensing water vapour in the atmosphere onto a cold surface. However, cooling a surface requires substantial energy, making the process not sustainable. We report the design and application of porous paint-like films made of poly(vinylidene fluoride-co-hexafluoropropylene)(PVDF-HFP) that passively cool when exposed to the sky, even under sunlight. The phase separation mechanism leading to pore formation was tuned by controlling ambient humidity, composition and thickness. The surface of the porous films was modified with a smooth topcoat to increase the roll-off of condensed water droplets. This paint-like coating gives access to the vast amount of water that is contained in the atmosphere and yields as high as 350 ml/m²/day have been achieved. Our approach requires no input of energy and could be applied on existing surfaces to provide a sustainable, delocalized source of water.

Energy-Efficient Catalysts For Green Ammonia Synthesis

Franck Natali^{1,2*}, Anna Garden³, Jay Chan², Caitlin Casey-Stevens¹, Mohsen Maddah², Sherry Xu², Pauline Calloch², and Paul Geraghty²

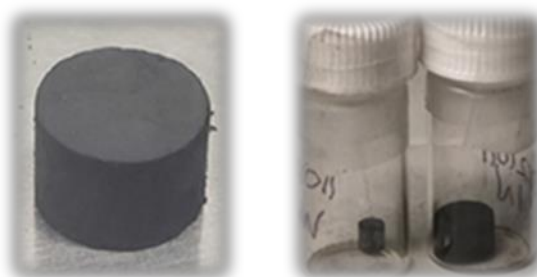
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Transitioning the “Hard-to-Abate” sectors like aviation, shipping, steel, cement, fertilisers towards zero CO₂ and greenhouse emissions has been extremely challenging. These sectors are the massive carbon emitters due to their enormous use of natural gases and crude fossil fuels. Amongst them, ammonia, an essential ingredient for nitrogen-based fertiliser, is responsible for ~2% of total energy consumption. The science problem is that reacting nitrogen and hydrogen form ammonia in the 115-year-old Haber-Bosch process is inefficient, energy-intensive, and requires high temperatures (>400°C) and pressure (>200 bar). Research to address these issues focuses primarily on reducing carbon emissions via alternative extraction methods for hydrogen, electrochemical ammonia synthesis, or catalyst developments, to cite but a few examples.

Despite several attempts, a simple catalyst material for widespread implementation of low-temperature/-pressure ammonia synthesis remains a challenge.¹⁻² In this presentation, we combine an experimental study with advanced computational investigations to show that lanthanide surfaces can break molecular nitrogen at ambient temperatures and pressures <1 bar with facile desorption – a remarkably simple catalyst approach that easily cleaves the strong nitrogen-nitrogen bond and more importantly releases the intermediate and final ammonia species.³⁻⁷

In addition, key fundamental features, activation energy and reaction orders derived from experimental kinetic studies will be presented, highlighting the low activation energy as well as the reduced hydrogen poisoning of our lanthanide catalyst powders and pellets. Finally, computational investigations (ab initio molecular dynamics and density functional theory) to investigate the atomic-scale mechanism of the ammonia formation reaction will be discussed.



Lanthanide catalyst pellets –
millimetres, 10 millimetres in

millimetres, 10 millimetres in height, respectively.

Dimensions: 5
diameter, and 5

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Catalytic high-entropy low melting point metal nanodroplets

Post-transition metals, especially those with low melting points such as gallium, indium, and their alloys, can be shaped into nanoscale droplets, possessing unique dynamics, fluidity, and surface properties fundamentally different from their solid forms.¹ These alloys can be alloyed with a broad spectrum of elements, including transition, noble metals and rare earth elements.²⁻⁴ By leveraging the properties of post-transition metal alloys to dissolve numerous elements, we introduce the concept of pseudo high-entropy liquid metal alloys at the nanoscale in liquid and solid forms (see figure). These alloys exhibit exceptional entropy levels and potential for enhanced catalytic applications, especially with noble metal atomic dispersion.

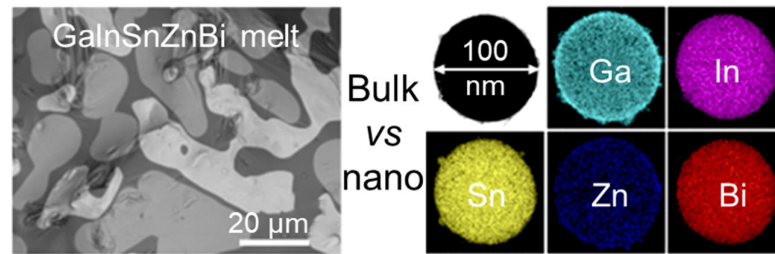
The formation, characteristics, and catalytic potentials of these novel high-entropy and multielemental nanoalloys was investigated. Nanoscale pseudo high-entropy alloys using gold, copper, platinum, and palladium in a gallium-indium solvent were synthesized. Another set of high-entropy post-transition metals consisted of tin, bismuth, indium, gallium, and zinc. These alloys demonstrated distinctive catalytic abilities, notably for hydrogen evolution reaction and CO₂ conversion.

Multiple metals were solvated at room temperature with enhanced atomic dispersion. In hydrogen evolution reactions, atomically dispersed platinum in GaIn-AuCuPtPd alloys showed improved catalytic activity in contrast to other systems.

The nanoscale pseudo high-entropy liquid metal alloys, exceeded the entropy of solid high-entropy alloys at room temperature. These novel nanodroplets prevent multiphase segregation and showcase enhanced catalytic activity, especially with atomic dispersion of platinum. This exploration opens vast possibilities for incorporating diverse elements, broadening the potential of high-entropy metal systems.



Nanoscale high-entropy homogenisation



Noble metal catalysts

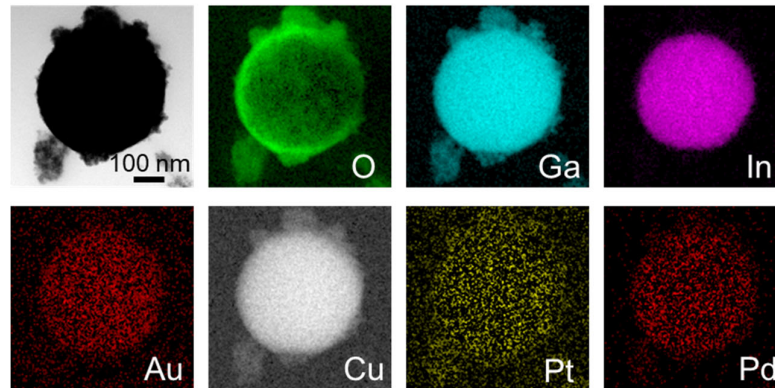


Figure 1. Back-scattered phase contrast SEM image of the solidification patterns of a bulk GaInSnZnBi alloy and TEM image and EDS mapping of a GaInSnZnBi nanoparticle. TEM image and EDS mapping of catalytic noble metal high-entropy nanoalloys. Preliminary data.

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Materials for the hydrogen economy

Hydrogen in the form of water is an abundant and effective potential fuel source. It is the most energetic by weight and produces water as a by-product. It has the potential to store renewable energy at greater scales and lower cost than any existing technologies. As a pure molecule or combined with other elements, hydrogen has the flexibility to address the needs of many sectors and the transition to decarbonised economies.

This presentation will discuss the roles of hydride materials as key enabler of the hydrogen economy, not only for storing hydrogen at scale, but also for hydrogen compression and purification. In particular, recent findings on reversibility paths in several high-capacity hydrogen storage materials and the implications of these findings will be discussed. This work brings hope that ways to design hydrogen release/uptake mechanisms from high-capacity complex hydrides are feasible as well as new applications toward advanced hydrogen technologies.





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Design of Scalable Nanoscale Electrocatalysts for Green Hydrogen and E-Fuels Production

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. 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 scalability as global energy carrier.

Here, 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 electrolyzers. 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 electrolyzers. 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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Liquid metal-based atomically thin doped materials for energy harvesting

Ultrathin materials, which are only a few atoms thick, have attracted significant attention due to their exceptional electrical, optical, and mechanical properties. The liquid metal-based reaction route using low melting point metals such as Ga, Sn, Bi, In, and their alloys, provides a unique technique for the fabrication of large area atomically thin materials from the interface of liquid metals.^{1, 2} This method enables access to numerous ultrathin materials that are not intrinsically layered and therefore cannot be produced as atomically thin layers using conventional methods.^{3, 4} This research aims to utilise the liquid metal approach for the controlled synthesis and doping of atomically thin materials with broken inversion symmetry and ferroelectric properties for energy harvesting applications.

Ultrathin ferroelectric materials including PbO and (Hf_{0.5}Zr_{0.5})O₂-doped SnO monolayers are harvested through a liquid metal touch-printing process which involves van der Waals exfoliation from the surface of liquid Pb and Sn-Hf-Zr alloys to a transfer substrate, respectively. An atomically thin layer of metal oxide grows on the surface of liquid metal at ambient oxygen. The interfacial oxide layer is effectively transferred to the substrate due to minimal interaction between liquid metal and surface oxide layer, and strong van der Waals interactions between the transfer substrate and surface oxide.¹

The generated atomically thin PbO and (Hf_{0.5}Zr_{0.5})O₂-doped SnO sheets exhibited significant piezoelectric coefficients of 30 and 10 pm/V, respectively.^{5, 6} In summary, The liquid metal synthesis technique can feasibly be used for harvesting and selective doping of ultrathin planar structures with extensive applications in energy harvesting, sensing, optics and electronics.

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Addressing Environmental Sustainability in Wind Energy: Recycling Composite Materials in Wind Turbine Blades

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Carbon Fibre Reinforced Polymer (CFRP) is a versatile anisotropic composite which plays a vital role in renewable energy and various industries. Its exceptional properties, such as high tensile strength, lightweight structure, and corrosion resistance, have made it suitable for the applications in renewable energy sector. However, the soaring global demand for CFRP has resulted in a concerning amount of waste, poised to reach 20 kilotons annually within the next two years. Projections indicate that over the next decade, there will be a cumulative generation of 15,000 tonnes of composite waste from discarded turbine blades, with an expected annual production of approximately 4,000 tonnes by 2034. This non-biodegradable waste poses a significant environmental threat when improperly disposed of in landfills. To address this pressing issue, this study proposes an environmentally sound solution - the establishment of a closed-loop life cycle for CFRP composites. Central to this approach is the development of efficient recycling methods aimed at separating carbon fibres from the composite matrix and reclaiming valuable fibres. This process not only mitigates the risks associated with landfill disposal but also reduces energy consumption in the production of virgin carbon fibres. Moreover, the study incorporates innovative CFRP surface pre-treatment techniques to ensure the recovered carbon fibres maintain their mechanical properties, maximising the economic value of recycled carbon fibre. By focusing on these critical aspects, this research contributes to sustainable wind energy practices. Additionally, it promotes a greener future by addressing the efficient recycling of carbon fibres, which not only mitigates the risks associated with landfill disposal but also reduces energy consumption in the production of virgin carbon fibres.



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Dynamic configurations of metallic atoms in the liquid state for selective propylene synthesis

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Dynamic configurations of metallic atoms in the liquid state for selective propylene synthesis

The use of liquid gallium as a solvent for catalytic reactions has enabled access to well dispersed metal atoms configurations, leading to unique catalytic phenomena, including activation of neighboring liquid atoms and mobility-induced activity enhancement. To gain mechanistic insights into liquid metal catalysts, here we introduce a $\text{GaSn}_{0.029}\text{Ni}_{0.023}$ liquid alloy for selective propylene synthesis from decane. Due to their mobility, dispersed atoms in a Ga matrix generate configurations where interfacial Sn and Ni atoms allow for critical alignments of reactants and intermediates. Computational modelling, corroborated by experimental analyses, suggests a particular reaction mechanism, by which Sn protrudes from the interface and an adjacent Ni, below the interfacial layer, aligns precisely with a decane molecule facilitating propylene production. We then apply this reaction pathways to canola oil attaining propylene selectivity of ~94.5%. Our results offer a mechanistic interpretation of liquid metal catalysts with an eye to potential practical applications of this technology.

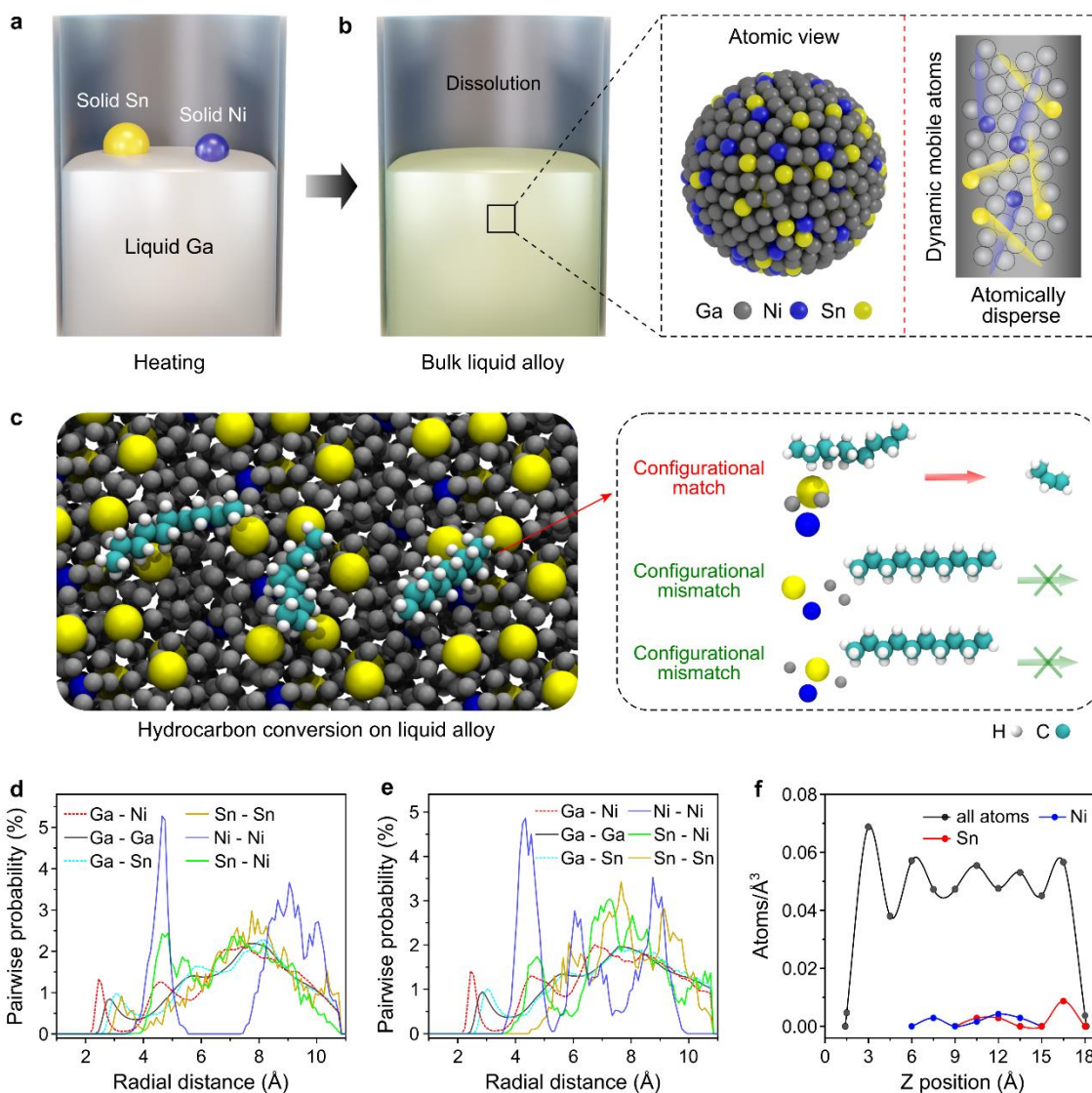


Fig. 1 | Schematics and computational simulations describing the $\text{GaSn}_{0.029}\text{Ni}_{0.023}$ catalyst and the configurational alignment enabled selective reactions. a,b, Schematics demonstrating the preparation (a) and the atomic mobility (b) of liquid $\text{GaSn}_{0.029}\text{Ni}_{0.023}$ catalyst. **c**, Schematics illustrating that one precise configurational alignment between the hydrocarbon and dispersed atoms in a Ga matrix initiated the selective reaction. **d,e**, Pairwise probability function for Ga, Sn, and Ni atoms in the bulk (d) and at the interfaces (e) of a $\text{GaSn}_{0.029}\text{Ni}_{0.023}$ catalyst. **f**, Atomic density profiles for all atoms, Sn, and Ni as a function of z position in the interfacial system at 100 ps.



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Design and development of nanomaterials for removal of emerging categories of persistent organic pollutants in contaminated water

The threat of antimicrobial resistance (AMR) is one among the top ten public health issues faced by world today as per the press release by World health organization (WHO) on 17th November 2021¹. The pressing issue cannot be solved without considering the increasing quantity of bio-recalcitrant organic compounds especially pharmaceutical wastes in our water bodies which is a direct consequence of the population blast as well as over usage of pharmaceutical drugs². Frequent consumption of antibiotics for human, veterinary and agricultural purposes has led to the incessant release of antibiotics to water resources and other similar environments resulting in a widespread invasion of antibiotic resistant bacteria (ARB) and antibiotic resistant gene (ARG) into water streams. We adopt Photo Fenton-process for antibiotic removal using passivation-bypassed Fe-alloy, rate-controlled using photo-activity. A simple but efficient method is proposed towards solar driven, compensated and coupled Fenton-photocatalysis process for the effective inactivation of antimicrobials in artificially contaminated waterbodies. Introduction of such processes are expected to open up new avenues for water treatment. Various Photoactive materials have also been designed for decontaminating water under light simultaneously producing power from wastewater through an efficient Photocatalytic Fuel Cell. Besides this, another approach on chemical immobilization of nano-photocatalysts using polymer matrix membranes for promising multicycle industrial wastewater treatment will also be discussed. A combination of these approaches can produce a number of tunable materials that can be investigated for applications spanning from energy to environmental remediation.

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