



EcoMat Conference 2024

July 8-10, 2024 Newcastle upon Tyne, UK



Welcome Letter

Dear Friends and Colleagues,

It is our great pleasure to welcome you to the EcoMat Conference, being held between 08-10 July 2024 organized by Northumbria University at Newcastle upon Tyne, UK

EcoMat Conference 2024 aims to host a face-to-face platform between scientists in academia and industry as well as policy makers around the world to exchange interdisciplinary ideas and expertise on the ever-changing environment. The objective is to bring together experts from academic institutions, industries and research organizations and professional engineers for sharing of knowledge, expertise and experience in the emerging trends related to life-changing materials research with the applications in renewable energy, circular economy and sustainable future.

Best regards, EcoMat 2024 Committee

2

EcoMat 2024 Conference Committee

Organizing Committee

Conference Chair Professor Ben Bin Xu (Northumbria University, UK)

Deputy Chair Professor Ximin He (UCLA, US)

Deputy Chair Professor Zijian Zheng (Hongkong PolyU, Chair of EcoMat conference series, HK)

Secretary Committee Member Committee Member Committee Member Committee Member Dr Muhammad Wakil Shahzad Dr Terence Liu Dr Sherry Chen Dr Yifan Li Dr Yunhong Jiang Professor Martin Birkett



Outline

- 1. Overview
- 2. About EcoMat Journal
- 3. Energy, Materials and Engineering Research at Northumbria University
- 4. Sponsors and Acknowledgement
- 5. Traffic and Map for conference
- 6. Short Programme
- 7. Awards and Bursary
- 8. Plenary Speakers (bio and abstract)
- 9. Researcher Award Winners
- 10. Abstracts
- Safety notes
- Things to do at Newcastle upon Tyne

Overview

The EcoMat Conference 2024 is organized by Northumbria University and hosted in Hilton Gateshead at Newcastle upon Tyne, UK, on 8th - 10th July 2024.

Parallel sessions will be focusing on the following topics:

- Symposium A: Catalysts and Catalysis
- Symposium B: Energy Storage
- Symposium C: Gas/Water Management and Circular Economy
- Symposium D: Harvesting, Conversion and Applications of Thermal/Wind/Solar/Hydrogen Energy
- Symposium E: Harvesting and Transformation of Mechanical & Biological Energy
- Symposium F: Smart Soft Materials for Energy and Environmental Application

About EcoMat



FUNCTIONAL MATERIALS FOR GREEN ENERGY AND ENVIRONMENT

Aim and Scope

EcoMat is an interdisciplinary journal uniting research on functional materials for green energy and environments. *EcoMat* aims to publish on a wide variety of topics from different disciplines that share the focus on cutting-edge advanced materials for green energy and environment. The scope of *EcoMat* is intentionally broad



and encompasses relevant fields for developing ecofriendly and sustainable energy, including topics such as wind, water and solar energy harvesting & conversion, batteries and supercapacitors, energy system and networks, thermoelectrics, fuel cells, carbon capture and storage, piezo and triboelectrics, water and air pollution control & cleaning, artificial photosynthesis, hydrogen generation & storage. This journal recognizes the complexity of issues, and therefore particularly welcomes innovative interdisciplinary research with wide impact. It will aim to make a mark in the materials science and adjacent fields with ambitions of a high academic impact.

Impact

2023 Journal Impact Factor: **10.7** Five-year Journal Impact Factor: **12.3** 2023 CiteScore: **17.3**

For more details, visit *EcoMat* website <u>http://www.wileyonlinelibrary.com/journal/ecomat</u>

Engineering is everywhere, from the buildings we live and work in to the products we use every day. Mechanical and Construction Engineering at Northumbria explores a wide range of areas, including research into advanced materials, product development, environment and energy, and many more.

Smart Materials & Surfaces Laboratory (SMSL) group is working on advance materials development. Smart materials and surfaces are ones designed with particular properties and whose properties can be changed by external forces or interfacial interactions. SMSL research group design and research into novel functional/structural materials and fabrication strategies, often at micro/nano scales, to investigate into liquid-solid interactions and development of smart devices employing smart materials and surfaces. The group conducts fundamental and applied sciences for various applications in energy materials, sensors, healthcare wearables, acoustofluidics. SMSL use novel functional/structural materials and fabrication strategies, such as directed assembly of complex, nano- and micro-constructed soft materials, hybrid nano- and microfabrication methods, and embroidery for smart textiles.

SMSL's recent research has been conducted in collaboration with a range of UK and international universities and with the support of the UK Engineering & Physical Sciences Research Council (EPSRC), Innovate UK, The Royal Society, European Commission, and industrial partners. SMSL lead Special Interest Groups (SIGs) on "Droplet and Flow Interactions with Bioinspired and Smart Surfaces" in the EPSRC-funded UK Fluids Network (UKFN).

The other research groups include Engineering Materials Mechanics Group, Fluid and Thermal Engineering, and Renewable Energy Technologies

For more information, please visit our webpage: <u>https://www.northumbria.ac.uk/about-us/academic-</u> <u>departments/mechanical-and-construction-engineering/research/</u>





Northumbria University NEWCASTLE











材料化学工程国家重点实验室 State Key Laboratory of Materials-Oriented Chemical Engineering



Hilton Gateshead overlooks the Tyne Bridge and are less than a mile from Gateshead metro station and eight minutes from the A1 motorway. The Quayside area is a short walk away, home to nightlife hotspots, Sunday markets, and art exhibitions. Utilita Arena and St James' Park are within two miles.

The hotel address: Bottle Bank, Gateshead, NE8 2AR, United Kingdom

Getting to Hilton Gateshead

From the Newcastle International Airport

- 1.1 By Metro Transit Railway (Metro): Take the Metro from Newcastle International Airport to Gateshead, then walk for 10 min. Fee: less than GBP £ 5; Transit time: ~40 minutes
- 1.2 By bus: Please check Google map. Fee: less than GBP £ 5; Transit time: ~40 minutes
- 1.3 By Airport Taxi: Fee: ~ GBP £ 30; Transit time: ~20 minutes

From the Newcastle Central Train Station

- 2.1 By Metro Transit Railway (Metro): Take the Metro from Newcastle Central Station to Gateshead, then walk for 10 min. Fee: less than GBP £ 3; Transit time: ~15 minutes
- 2.2 By Walking: Please check Google map, Fee: GBP £ 0; Transit time: ~15 minutes
- 2.3 By Taxi: Fee: ~ GBP £ 15; Transit time: ~15 minutes



Conference Map – Hilton Layout



*Please check here for a Full Map for Hotel Gateshead.

Short Programme

07 July 2024 (Sunday)			
14:00 - 19:30	Registration (Hilton Gateshead Suite Foyer)		
17:30 - 19:30	Welcoming drink for all (Hilton Gateshead Suite Foyer)		
08 July 2024 (Monday)			
all day Registration (Hilton Gateshead Suite Foyer)			
08:30 - 08:45	Opening Ceremony by Prof.Zijian Zheng and Conference Chair (Hilton Gateshead Suite)		
08:45 - 09:45	P-1 Prof. Zaiping Guo - The University of Adelaide, AU (Hilton Gateshead Suite)		
09:45- 10:45	P-2 Prof. Yi Cui - Standford University, US (Hilton Gateshead Suite)		
10:45- 11:10	Coffee Break & Group Photo (Hilton Gateshead Suite Foyer)		
11:10- 12:10	P-3 Prof. Guihua Yu - UT Austin, US (Hilton Gateshead Suite)		
12:10 - 13:10	P-4 Prof. Esther T. Akinlabi - Northumbria Univeristy, UK (Hilton Gateshead Suite)		
13:10 - 14:00	Lunch Break & Poster session & Technical demo (Hilton Gateshead Suite Foyer)		
14:00 - 15:50	Symposium A Symposium B Symposium B Session 1 (BR1) Session 1 (BR2) Session 1 (MR2)	C Symposium D Symposium E Symposium F R1) Session 1 (BR3) Session 1 (MR2) Session 1 (MR3)	
15:50 - 16:10	Coffee Break (Hilton Gateshead Suite Foyer)		
16:10 - 17:20	Symposium A Symposium B Symposium B Session 2 (BR1) Session 2 (BR2) Session 2 (MR2)	C Symposium D Symposium E Symposium F R1) Session 2 (BR3) Session 2 (MR2) Session 2 (MR3)	
17:20 - 18:30	Poster session(Hilton Gateshead Suite Foyer)/Dinner	Reception for Speakers hold by Symposium Chairpersons	
9 July 2024 (Tuesday)			
08:30 - 09:30	:30 P-5 Prof. Xuanhe Zhao - MIT, US (Hilton Gateshead Suite)		
09:30- 10:30	P-6 Dr. Khalil Amine - Argonne National Laboratory, US (Hilton Gateshead Suite)		
10:30- 10:45	Coffee Break (Hil	ton Gateshead Suite Foyer)	
10:45 - 12:35	Symposium A Symposium B Symposium B Session 3 (BR1) Session 3 (BR2) Session 3 (M	C Symposium D Symposium E Symposium F R1) Session 3 (BR3) Session 3 (MR2) Session 3 (MR3)	
12:35 - 14:00	Lunch Break & Poster session & Te	Lunch Break & Poster session & Technical demo (Hilton Gateshead Suite Foyer)	
14:00 - 15:45	Editor Forum, BR1 Thematic session		
15:45 - 16:00	Coffee Break (Grab&Go type, Hilton Gateshead Suite Foyer)		
18:15 - 21:30	Conference Banquet and Researcher Awards Ceremony (Hilton Gateshead Suite/BR1-3)		
10 July 2024 (Wednesday)			
09:00 - 11:00	EcoMat Researcher Awards Lectures (Hilton Gateshead Suite)		
11:00 - 11:15	Coffee Break (Hilton Gateshead Suite Foyer)		
11:15 - 12:35	Symposium A Symposium B Symposium B Session 4 (BR1) Session 4 (BR2) Session 4 (M	C Symposium D Symposium E Symposium F R1) Session 4 (BR3) Session 4 (MR2) Session 4 (MR3)	
12:35 - 14:00	Lunch Break & Technical	Jemo (Hilton Gateshead Suite Foyer)	
14:00 - 15:00	Symposium A Session 5 (BR1)	Symposium E Session 5 (MR2)	
15:00 - 15:15	5:00 - 15:15 Coffee Break (Grab&Go type, Hilton Gateshead Suite Foyer)		
15:15 - 15:40	Presentation Awards and Closing Remarks (Hilton Gateshead Suite)		

Please download the conference programme PDF at the section of 'resource' here.



We are proud to announce the recipients of this year's EcoMat awards, celebrating outstanding contributions and achievements in the field of Material Science. These awards recognize individuals and teams whose work has demonstrated exceptional innovation, dedication, and impact.



- EcoMat Young Researcher Award Two researchers will be selected. The award recipients will be presented with an award certificate/trophy and a cash prize of \pounds 500.
- EcoMat Mid-career Researcher Award one researcher will be selected. The award recipient will be presented with an award certificate/trophy and a cash prize of \pounds 1000.
- There will be a number of oral presentation and poster awards, which will be assessed by the award committee.

Oral & Poster award

EcoMat 2024 will have multiple *Oral & Poster awards*, the outcome will be unveiled during the conference.

Plenary Speakers



Professor Khalil Amine Argonne National Laboratory, USA



Professor Yi Cui Stanford University, USA



Professor Esther Akinlabi Northumbria University, UK



Professor Zaiping Guo The University of Adelaide, Australia



Professor Xuanhe Zhao MIT, USA



Professor Guihua Yu The University of Texas at Austin, USA

Plenary Speakers Bio and Abstracts

Professor Zaiping Guo



She is an Australian Laureate Fellow at School of Chemical Engineering, The University of Adelaide. She received her PhD from University of Wollongong in 2003 and was elected to Fellow of the Australian Academy of Science and the Australian Academy of Technological Sciences and Engineering in 2023. Her research focuses on the design and application of electrode materials and electrolyte for energy storage and conversion, including rechargeable batteries, hydrogen storage, and fuel cells. Her research achievements have been recognized through numerous awards, including an ARC

Queen Elizabeth II Fellowship in 2010, an ARC Future Professorial Fellowship in 2015, an ARC Laureate Fellowship (2021), and the Clarivate Analytics Highly Cited Researcher Award in 2018, 2019, 2020, 2021, and 2022. Furthermore, in 2020, she was honoured with the NSW Premier's Prizes for Science & Engineering, specifically for her outstanding achievements in Engineering or Information and Communications Technology.

Electrode and electrolyte design for high-performance aqueous zinc-ion batteries

Jianfeng Mao, Sailin Liu, Yanyan Wang, Jodie Yuwono, Shilin Zhang, Zaiping Guo School of Chemical Engineering, The University of Adelaide, Adelaide, SA 5005, Australia Email: <u>zaiping.guo@adelaide.edu.au</u>

The rise of intermittent renewable sources, such as solar and wind, has spurred growing interest in electrical energy storage. Integrating grid-scale energy storage with renewable sources offers significant advantages in energy regulation and grid security. Zinc-based aqueous batteries (ZABs) have emerged as a promising energy storage technology for low-cost and large-scale applications due to the intrinsic safety of aqueous electrolytes and the highly desirable properties of the zinc metal anode, including its high theoretical capacity (820 mA h g⁻¹ and 5855 mA h cm⁻³), low redox potential, and abundant resources. However, the practical application of ZABs has faced challenges, including cathode degradation, uncontrollable zinc dendrite growth, and parasitic side reactions between the electrode and electrolyte, particularly under harsh conditions. In this presentation, I will discuss some of our recent advancements in enhancing the electrochemical performance of aqueous zinc ion batteries through electrode design and electrolyte optimization.

Professor Yi Cui



He is the Fortinet Founders Professor of Materials Science & Engineering and Energy Science & Engineering at Stanford University. He was the Director of the Precourt Institute for Energy and is the founding Director of Sustainability Accelerator at Stanford. He is known for reinventing batteries through nanoscience and has also made broad contributions on 2D materials, topological quantum materials, catalysts, thermal textile, water and air purification, and cryoEM. He is an elected member of the US NAS and European Academy of Engineering. He is a fellow of the American Academy of Arts & Sciences, Materials Research Society,

Electrochemical Society, and the Royal Society of Chemistry. He has been recognized with the Global Energy Prize, U.S. Department of Energy's Lawrence Award, MRS Medal, and Blavatnik National Laureate. He has founded five companies to commercialize technologies from his group: Amprius (NYSE: AMPX), 4C Air, EEnotech, EnerVenue and LifeLabs Design

Reinventing Batteries Through Materials Design

Stanford University Email: vicui@stanford.edu

This talk presents two decade long research in my lab on materials design for reinventing batteries to revolutionize next generation of electric mobility and stationary energy storage, including 1) Silicon anodes; 2) Li metal anodes; 3) Sulfur cathodes; 4) Newly designed fluorinated electrolytes, suspension electrolytes and high entropy electrolytes for improving cycling coulombic efficiency; 5) Studying corrosion and capacity fading mechanisms leading to designing strategies for the recovery of isolated Li metal; 6) Novel technique developments for understanding batteries, including cryogenic electron microscopy and electrochemical techniques. 7) Aqueous batteries for grid-scale energy storage

Professor Guihua Yu



He is a Temple Foundation Professor of Materials Science and Mechanical Engineering at The University of Texas at Austin. His research has broadly centered on nanomaterials innovation for advanced energy, environment, and sustainability technologies. Yu is a Fellow of MRS, RSC, IOP, and IAAM, and has been consistently ranked among one of the Top Highly Cited Researchers in both Materials Science and Chemistry fields by Web of Science. He has received many prestigious international/national

awards and honors for research and education, including Blavatnik National Awards Honoree, RSC Horizon Prize, Norman Hackerman Award in Chemical Research by The Welch Foundation, Edith and Peter O'Donnell Award by Texas Academy of Medicine, Engineering and Science (TAMEST), TMS Brimacombe Medalist Award, Polymer International-IUPAC Award for Creativity in Applied Polymer Science, Camille Dreyfus Teacher-Scholar Award, Sloan Research Fellow, *MIT Technology Review* 'Top Innovators Under 35' global list. Yu currently serves as Associate Editor of *ACS Materials Letters* (a flagship materials science journal by ACS), and Advisory/Editorial Board Member of over 20 international scientific journals.

A Soft Material Paradigm Towards Grand Energy-Water Nexus Challenges Temple Foundation Professor of Materials Science, Mechanical Engineering Texas Materials Institute, UT Energy Institute, The University of Texas at Austin Email: <u>ghyu@austin.utexas.edu</u>

Energy and water are of fundamental importance for our modern society, and advanced technologies on sustainable energy storage and conversion as well as water resource management are in the focus of intensive research worldwide. Beyond their traditional biological applications, hydrogels are emerging as a powerful material platform for energyand water-related applications owing to their attractive and tailorable physiochemical properties. This talk will present an emerging class of polymeric materials we have developed in the past decade: nanostructured multifunctional hydrogels that are hierarchically porous, and structurally tunable in size, shape, composition, hierarchical porosity, and chemical interfaces. These organic gels based on versatile gelation chemistries with highly tunable molecular building blocks offer an array of advantageous features such as intrinsic 3D nanostructured conducting frameworks, exceptional electrochemical activity to store and transport ions, and synthetically tunable polymer-water interactions.

We have demonstrated this new class of 'energy gels' to achieve a number of appealing functions that enable them to address key challenges in sustainable energy-water nexus. Several examples on functional organic gels-enabled advanced energy-water-related applications such as high-efficiency energy storage and conversion systems, solar water desalination and atmospheric water harvesting, and sustainable agriculture technologies, will be discussed to illustrate 'structure-derived multifunctionality' of this emerging class of materials.

Professor Esther Akinlabi



She is a Professor of Mechanical Engineering and serves as Deputy Faculty Pro Vice Chancellor for Research and Knowledge Exchange in Faculty of Engineering and Environment, Northumbria University, UK. She previously served as the Director of Pan African University Life and Earth Sciences Institute (PAULESI), Ibadan, Nigeria. Prior to joining PAULESI, she had a decade of meritorious service at the Department of Mechanical Engineering Science, University of Johannesburg (UJ), South Africa. At UJ, she served as the Head of Department of

Mechanical Engineering Science and as Vice Dean for the Faculty of Engineering and Built Environment. Her research interests are modern and advance manufacturing processes. She is a Fellow of the African Academy of Science (FAAS) and Fellow of the Nigerian Academy of Science (FAS).

Circular Plastic Economy (Waste to Wealth): Fostering Innovation and Entrepreneurship

Esther T. Akinlabi¹, Muyiwa Oyinlola² and Adedapo Adedeji³ ¹Department of Mechanical and Construction Engineering, Northumbria University, UK ²Department of Mechanical Engineering, De Montfort University, Leicester, UK ³Pan African University, Life and Earth Sciences Institute, Ibadan, Nigeria Email: esther.akinlabi@northumbria.ac.uk

This project was aimed at demonstrating how universities can drive a thriving ecosystem for innovation and entrepreneurship in the circular plastic economy (waste to wealth). The objectives of the project were to foster a thriving ecosystem for innovation and entrepreneurship, build capacity and create an enabling environment for innovations and to organise, strengthen and enable an ecosystem with the goal of adding value to circular plastic economy. The circular plastic economy was demonstrated using plastic waste from bottled water which were collected, grounded, fed through an extrusion system for melting and filament were produced for 3D printing of many products.



Professor Xuanhe Zhao



He is a Professor of Mechanical Engineering at MIT. The mission of Zhao Lab is to advance science and technology between humans and machines to address grand societal challenges in health and sustainability. A major focus is the study and development of soft materials and systems. Dr. Zhao has won early career awards from NSF, ONR, ASME, SES, AVS, Adhesion Society, JAM, EML, and Materials Today. He is a Clarivate Highly Cited Researcher. Bioadhesive ultrasound, based on Zhao Lab's work published in Science, was named

one of TIME Magazine's Best Inventions of the year in 2022. SanaHeal Inc., based on Zhao Lab's work published in Nature, was awarded the 2023 Nature Spinoff Prize. Over ten patents from Zhao Lab have been licensed by companies and have contributed to FDA-approved and widely-used medical devices.

Merging Humans and Machines with Biopolymers: Innovation and Translation Xuanhe Zhao Massachusetts Institute of Technology

Whereas human tissues and organs are mostly soft, wet, and bioactive, machines are commonly hard, dry, and abiotic. Merging humans and machines is of imminent importance in addressing grand societal challenges in health, sustainability, security, education, and happiness of living. However, merging humans and machines is extremely challenging due to their fundamentally contradictory properties. At MIT Zhao Lab, we invent, understand, and facilitate the translation of soft materials based on biopolymers to form long-term, robust, non-fibrotic, and high-efficacy interfaces between humans and machines. In this talk, I will discuss two examples of merging humans and machines with biopolymers. I will propose two challenges in science and technology:

· Can we develop fully non-fibrotic implants?

• Can we image the whole body continuously over days to months?

I will conclude the talk with a vision for future human-machine convergence – aided by and synergized with modern technologies such as artificial intelligence, synthetic biology, and precision medicine.

Dr. Khalil Amine



He is an Argonne Distinguished Fellow and the leader of the Advanced Battery Technology team at Argonne National Laboratory, where he is responsible for directing the research and development of advanced materials and battery systems. He serves as a member of the US National Academy of inventors and fellow of the European academy of sciences and committee member of the U.S. National Research Consul at US Academy of Sciences on battery related technologies. Dr. Amine is 2023 recipient of Kuwait prize, 2019 recipient of the mega global energy prize, 2013 DOE Vehicle technologies office award and is the

six-time recipient of the R&D 100 Award. He is also the chairmen of the international automotive lithium battery association, ECS fellow, Fellow of the international association of advanced materials, and associate editor of the journal of Nano-Energy.

Advanced Lithium-ion Battery and Beyond for Enabling Mass Electrification of Vehicles

<u>K. Amine</u> Argonne National Laboratory, 9700 South Cass Av., Argonne, IL <u>Email: amine@anl.gov</u>

To meet the high-energy requirement that can enable the 40-miles electric drive Plug in Hybrid Electric Vehicle (P-HEVs), long range electric vehicle (EV) and smart grid, it is necessary to develop very high energy and high-power cathodes and anodes that when combined in a battery system must offer over 5,000 charge-depleting cycles, 15 years calendar life as well as excellent abuse tolerance. These challenging requirements make it difficult for conventional lithium-ion battery systems to be adopted in P-HEVs and EVs. In this talk, we will first describe the challenges and barriers that need to be overcome to achieve mass electrification of vehicles. We will then introduce the next generation lithium-ion battery that include Ni rich full gradient cathode coupled with an advanced cathode particle coating to improve life and sfety of this new battery system. We will also touch on high voltage and non-flammable Fluorinated based electrolytes and Silicon-graphene composite anode including a novel pre-lithiation technology to overcome the irreversible loss of this anode in the first cycle and increase significantly the energy density of the system. We will then finish by describing a novel lithium superoxide based close battery system that offer at least 2 times the energy density of the state-of-the-Art lithium ion battery and a low cost SeS₂₂ system with novel electrolyte that suppress the dissolution of polysulfide species and prevent the shuttle effect.



EcoMat Mid-career Researcher Award



Professor Lianzhou Wang (The University of Queensland, Australia)

Lianzhou Wang is professor and Australian Research Council (ARC) Australian Laureate Fellow in the School of Chemical Engineering, Director of Nanomaterials Centre, and Senior Group Leader of Australian Institute for Bioengineering and Nanotechnology, The University of Queensland (UQ), Australia. His research focuses on the design and application of semiconductor nanomaterials for renewable energy conversion and storage including photocatalysts for hydrogen production, low-cost solar cells and rechargeable batteries. Lianzhou has published > 600 peer-reviewed journal articles, and filed 19 patents, with a Hindex of 125. He won some prestigious honours/awards including the prestigious ARC QEII Fellowship (2006), Future Fellowship (2012), Laureate Fellowship (2019) and Industry Laureate Fellowship (2024), UQ Research Excellence Award & Research Supervision Award, Scopus Young Researcher Award, and Research Excellence Award in Chemical Engineering. Lianzhou serves as the Editor/Associate Editor/editorial board of more than 10 journals, and is the President of Australian Materials Research Society. He is a fellow of the Australian Academy of Science (FAA), Royal Society of Chemistry (FRSC) and Academia Europaea (MAE), and is named on the Clarivate' Highly Cited Researchers list.

• This award lecturer will be scheduled at 9:05 – 9:50 am, July 10th.



EcoMat Young Researcher Award



Professor Po-Chun Hsu (The University of Chicago, United States)

Po-Chun Hsu is an Assistant Professor at the Pritzker School of Molecular Engineering at the University of Chicago, focusing on light- and heat-managing materials for energy, sustainability, and health. He earned his PhD degree in Materials Science and Engineering and was a postdoctoral researcher in Mechanical Engineering, both at Stanford University. Prior to joining the University of Chicago, he was an Assistant Professor of Mechanical Engineering and Materials Science at Duke University from 2019 to 2022. He is a recipient of the NSF CAREER Award, shortlist for the Falling Walls Science Breakthrough of the Year 2023, Ralph E. Powe Junior Faculty Enhancement Awards, MIT Technology Review Innovators Under 35 (China), Clarivate Analytics Highly Cited Researchers, and Sony Faculty Innovation Award. His project in cooling textiles was selected as Top Ten World-Changing Ideas by Scientific American.

• This award lecturer will be scheduled at 9:50 – 10:25 am, July 10th.



EcoMat Young Researcher Award



Professor Paul McGonigal (The University of York, United Kingdom)

Professor Paul McGonigal is known for his research into dynamic processes in organic functional materials, spanning topics as diverse as aromatic cation materials, solid-state luminescence, self-assembled soft surfaces and fluxional molecules. He is a current recipient of an EPSRC Fellowship and an ERC Consolidator grant at the University of York, where his group's research has been recognised by the RSC Harrison–Meldola Memorial Medal (2022) and the Liebig Lectureship from the German Chemical Society (2023). Paul's training started with undergraduate (MChem, 2007) and postgraduate (PhD, 2011) degrees from The University of Edinburgh, working under the direction of Prof David Leigh. He moved to The Institute of Chemical Research of Catalonia, Spain, as a Postdoctoral Researcher (2011) in the laboratory of Prof Antonio Echavarren then went on to conduct research with Prof Fraser Stoddart's research group at Northwestern University as a US–UK Fulbright Scholarship (2012). Paul started his independent academic career at Durham University as an Assistant (2015) and Associate Professor (2021), before moving to the University of York as a Reader (2023) and then Full Professor (2024).

• This award lecturer will be scheduled at 10:25 – 11:00 am, July 10th.

General Guidelines

Preparation

- 1. **Content**: Ensure your presentation is clear, engaging, and tailored to your audience.
- 2. Slides: Use visuals to complement your talk. Keep text minimal and use large fonts.
- 3. **Practice**: Time your presentation to ensure it fits within the allocated slot.

Presentation

- 1. **Introduction**: Start with a brief introduction of yourself and the topic.
- 2. Structure: Outline your key points early.
- 3. Engagement: Be prepared to handle questions both during and after your talk.
- 4. Timing: Stick to the time limit. Respect the schedule and other speakers.

Time Allocation

Plenary Talk

- Total Duration: 55 minutes
 - Presentation: 45 minutes 0
 - **Q&A**: 10 minutes \circ
- Please send your presentation file (.PPT or PDF) to the conference email by July 7th • and bring your presentation on a USB drive/your personal laptop on the site.

Invited Keynote Talk (amber cell in the presentation programme, sample as below)

- Total Duration: 29 minutes
 - Presentation: 25 minutes
 - **Q&A**: 4 minutes

A5.1 XX presenter name XXX institution name XXX ABS XXX

- Please arrive 15 min before the starting of your session to upload and test the • presentation slides on conference facility, or you can send your presentation file (.PPT or PDF) to the conference email by July 7th.

Invited Talk (Green cell in the presentation programme, sample as below)

- **Total Duration**: 19 minutes
 - **Presentation**: 15 minutes B5.3 XXXXXX ABS XXX • **Q&A**: 4 minutes
- Please arrive 15 min before the starting of your session to upload and test the • presentation slides on conference facility, or you can send your presentation file (.PPT or PDF) to the conference email by July 7th.

Technical Requirements

- 1. Equipment: The venue will provide a laptop. Please ensure the compatibility of your presentation file (PowerPoint, PDF, etc.).
- 2. Files: Name your presentation file as 'ABSXXX-your last name'.
- 3. Video/Audio: If your presentation includes video or audio, test it beforehand to ensure it works seamlessly with the provided equipment.

Additional Tips

- 1. Dress Code: Business casual unless otherwise specified.
- 2. Feedback: Be open to feedback and use it to improve future presentations.

****Oral presentation awards will be announced at the closure remark session of conference (July 10th)

Guidelines for Posters

<u>Layout</u>

- Poster Size: A0 or A1
- Orientation: Portrait
- Margin: Minimum 20 mm on all sides

<u>Design Elements</u>

Title and Header

- **Title**: Bold, large font (minimum 72 pt for A0, 60 pt for A1). Centered at the top.
- Authors and Affiliations: Below the title, slightly smaller font (48 pt for A0, 36 pt for A1). Include names, affiliations, and contact information.

Sections

- Introduction: Brief background and objectives.
- Methods: Describe the methodology clearly.
- **Results**: Use charts, graphs, and images.
- **Discussion**: Interpret the results and their implications.
- Conclusion: Summarize key points.
- References: List key references.
- Acknowledgements: Recognize contributors and funding sources.
- Line Spacing: Ensure adequate line spacing for readability.

Practical Tips

- 1. **Consistency**: Use consistent formatting, colors, and styles throughout the poster.
- 2. Brevity: Use bullet points to present information clearly and avoid large blocks of text.
- 3. **Readability**: Ensure text is legible from a distance of 1-2 meters.

**Important Notes

- The poster should be put at the board with your ABS number.
- Poster presenters need be with their posters at the lunchtime and coffee sessions for July 8th and 9th (except Crab&Go coffee session at the afternoon of 9th).
- You need set up your poster before 10 am, July 8th.
- You need **take your poster off by 3 pm, July 9th.** Unclaimed poster at the end of conference will be shredded.
- The assessment of your poster will take place between 1pm, July 8th 3 pm, July 9th. The poster award will be announced at the conference banquet.



Editor's Forum



Lisa Smith obtained a Bachelor of Arts and Sciences with honours in chemistry at the University of Melbourne (Australia), followed by a PhD focused on nanoparticle synthesis. Since joining Wiley in 2010, she has worked across quite a range of Materials Science journals, as well as writing for Advanced Science News and the bee smart city blog. She is currently Deputy Editor for Small and Editorin-Chief of Nano Select.

<u>Editor-in-Chief of Nano Select</u> <u>Deputy Editor of Small</u> <u>Editor of Adv Energy Mater,</u> <u>Adv Mater Inter</u>



Editor-in-Chief of EcoMat

Zijian Zheng is currently a Chair Professor of Soft Materials and Devices at the Department of Applied Biology and Chemical Technology, Associate Director of the Research Institute of Wearable Intelligent Systems, and Associate Director of the University Research Facility in Materials Characterization and Device Fabrication at PolyU. He received his B. Eng. in Chemical Engineering at Tsinghua University in 2003 and Ph.D. in Chemistry at University of Cambridge in 2007. In 2008–2009, he worked as a Postdoctoral Research Associate with Prof. Chad A. Mirkin at the International Institute for Nanotechnology at Northwestern University. His research interests include surface and polymer science, nanofabrication, flexible and wearable electronics, and energy conversion and storage. He serves as Editor-in-Chief of *EcoMat* and served as Guest Editor of Advanced Materials and Small. He is an Editorial Board Member of Advanced Energy Materials (Wiley) and npj Flexible Electronics (Springer Nature). Prof. Zheng is elected

Founding Member of The Young Academy of Sciences of Hong Kong and Chang Jiang Chair Professor by the Ministry of Education of China.



Editor of Chem Sci (RSC)

Dr Esther Johnston is a Scientific Editor for *Chemical Science, the flagship journal of the Royal Society of Chemistry*. She joined the RSC in 2021 as a Publishing Editor and worked on *Journal of Materials Chemistry A, Green Chemistry, and Nanoscale before joining the Chemical Science* team in January 2023.

Esther obtained a PhD in bioinorganic chemistry at Stanford University, USA, working with Professor Edward Solomon, then did a post-doc at the University of York with Professor Gideon Davies and Professor Paul Walton. She used spectroscopy and computational chemistry to study copper-containing enzymes involved in industry and the environment.

Keynote ABSTRACTS

A1.1

Bottom-up Synthesis of Amphiphilic Janus Catalysts for Aerobic Oxidation of Aromatic Alcohols in Foams

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Gas-liquid-solid (G-L-S) multiphase reactions are ubiquitous in the chemical industry. Conventional G-L-S reactors such as packed beds and stirred reactors typically suffer from low gas solubility in liquids and mass transfer limitations due to spatial separation of the different phases.¹ An elegant solution to boost the G-L-S contact encompasses the design of catalysts that can adsorb at the G-L interface generating particle-stabilized foams.² Herein, we designed a new type of amphiphilic catalyst with Janus architecture by bottom-up synthesis and engineered an efficient foam system for the aerobic oxidation of aromatic alcohols. Janus silica particles (250nm) were synthesized by the Pickering emulsion template method,³ whereby 1H,1H,2H,2H-perfluorooctyltriethoxysilane/3-mercaptopropyltriethoxysilane were sequentially grafted on pristine silica. Also, randomly functionalized particles were synthesized by co-grafting of both precursors on silica. Next, Pd nanoparticles were immobilised on both particles yielding Pd/JPs and Pd/Non-JPs. The anisotropic distribution of organic moieties and Pd nanoparticles over Pd/JPs was confirmed by Photo-Induced Force Microscopy (PiFM) using the band at 1145 cm⁻¹ (C-F stretching) and TEM, respectively (**Figure 1a-e**).

Two catalytic tests were conducted over Pd/JPs and Pd/Non-JPs (1wt%) at 100 °C in benzyl alcohol (BnOH)/o-xylene (1:1 v/v) mixture using stirring speeds of 500 and 1500 rpm (**Figure 1f**). The benzaldehyde yield was only 10% for Pd/Non-JPs at both stirring speeds. In contrast, for Pd/JPs, the yield increased from 10% to 22% with concomitant formation of abundant foam. The kinetic profiles for Pd/JPs and Pd/Non-JPs revealed an increase of activity to 2 times for Pd/JPs at 1500 rpm (**Figure 1g**). We next extended the scope of our foam system to a variety of aromatic alcohols showing double activity for Pd/JPs compared to Pd/Non-JPs.

These results highlight how the fine synthesis of Janus particles can enhance the interfacial activity of catalysts in G-L-S reactions in foam. This work also shows the first example of the application of PiFM to elucidate the surface topology of Janus particles with an anisotropic distribution of organic moieties.



Figure 1. (a) FT-IR and (b) PiFM spectra of pristine silica, JPs and Non-JPs; Topography, PiFM at 1145 cm⁻¹, and TEM of (c) pristine silica, (d) JPs, and (e) Non-JPs; (f) Aerobic oxidation of BnOH over Pd/JPs and Pd/Non-JPs as a function of stirring speed (1 h reaction). (g) Kinetic profiles for Pd/JPs and Pd/Non-JPs at 1000 and 1500 rpm. Reaction conditions: 0.8 mL of BnOH, 0.8 mL of o-xylene, O₂ balloon, 1wt% particles, 100 °C.

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A1.2

A journey from carbonization to decarbonization

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Porous carbon materials represent an exciting family of functional carbonaceous materials for energy and environmental applications. Conventional porous carbons possess intrinsic structural stability, interconnectivity, and chemical tuneability, and are popularly used in devices as separators or chemically inert conductive supports. Our group has been active in the research on heteroatom-doped porous carbon membranes (HPCMMs) as electro(co)catalysts in energy devices. Synergy of the porous nature, incorporation of heteroatoms, and the membrane state creates a vivid profile pattern. The first part of the talk will summarize our progress in synthesis of porous carbon membranes via carbonization of polymeric templates. [1] In the second part, I will continue the talk by applying the as-made porous carbon materials in electrochemical reactions for fuel decarbonization techniques, e.g. water splitting,[2] electrochemical CO_2 reduction [3] and hydrazine oxidation reactions [4-6].

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A1.3

Metallated Graphynes: Synthesis, Characterization and Application Studies

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Graphynes are non-natural carbon allotropes associated with periodic acetylene linkages that involve a mixed hybridization of sp^n (1 < n < 2). However, related research work on the metallated graphynes is much less explored. In this talk, we will present an interesting family of metallated graphynes (MGYs) with different ligand structures (Fig. 1). Bottom-up nanosheets with different topological structures, pore sizes, surface areas and advanced functionalities (e.g. tunable optical, electronic and magnetic properties) can be prepared by different monomer combinations. It is shown that this new class of organometallic 2D nanomaterials can find applications in the fields of nonlinear optics and catalysis.



Fig. 1 Chemical structures of metallated graphynes (a) HgL1, (b) HgL2 and (c) Hg-CoTPP.

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A2.1

Mass Transfer Enhancement for Gas Diffusion Electrode Based Electrochemical Reactors

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The electrochemical reaction generally occurs at the interface between electrode/electrocatalyst and electrolyte including charge transfer, phase transformation and mass transport. These reactions involve charge transfer, phase changes, and mass transport. A major challenge in these reactions is the limited mass transfer, primarily due to the properties of liquid and gaseous reactants that have low concentrations on the electrode/electrocatalyst surface. This presentation will highlight various strategies designed to enhance mass transfer. These include modifying electrochemical reactors¹, using alternative electrodes², and altering the structure of the electrocatalyst layers³. These approaches can effectively lower reaction barriers, thereby achieving rates sufficient for the reactants to be present along the gas-liquid-solid interface. This shortens the gas diffusion path and enhances mass transfer. These techniques have been widely adopted in eCO2RR and fuel cell applications.

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A3.1

Advanced Atomic Catalysts Design for Energy Systems

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Currently, atomic catalysts (ACs) as the frontier research topics have attracted tremendous attention. To supply theoretical guidance for designing novel electrocatalysts, we have carried out a comprehensive mapping study of graphdiyne (GDY) based ACs. First, we have proposed the "Redox Barrier Model" to quantify the capability of electron exchange and transfer (ExT), which enables the comparison of different AC systems. For the hydrogen evolution (HER) process, we have extended the conventional indicator of proton binding energy to more diverse indicators including chemical binding energy, desorption energy, and electronic structures. For the first time, we have identified GDY-Eu and GDY-Sm as two promising electrocatalysts for HER, which are also verified by machine learning. For the developments of dual atomic catalysts (DACs), we have investigated the formation stability and electronic modulations for all the combinations between transition metals (TMs) and lanthanide (Ln) metals. Due to the electronic self-balance effects by f-d orbital coupling, the combinations between the Ln metals and TMs achieve optimized stability and electroactivity of GDY-DACs. Meanwhile, the introduction of the main group elements enables activations of the electroactivity of GDY. Recently, we have also achieved the applications of GDY-ACs for the CO₂ reduction reaction (CO₂RR) with a comprehensive reaction pathway mapping of C_1 and C₂ products for the first time, where different metal selections display distinct selectivity and reaction trends. We propose the integrated large-small cycle mechanism to explain the challenges for C₂ product generation and identify the double-dependence correlation with metal and active sites. First-principle machine learning predicts the reaction energy of C-C couplings, where the adsorptions of the intermediates are critical to achieving accurate predictions of multi-carbon products. Therefore, these theoretical explorations have supplied important theoretical insights into the applications of ACs, opening a new avenue for the rational design of ACs for different energy systems.

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A3.2

Beyond the Bulk: Modelling Interfaces and Ion Transport in Solid Electrolytes

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Ion transport is pivotal to the performance of energy technologies, particularly batteries, and therefore the journey to net-zero emissions. The materials that exhibit ion conduction in these technologies present stunning heterogeneity and a plethora of complicated ion diffusion mechanisms from which they often derive their functionality. This situation is further complicated when we begin to consider the nanostructures, microstructures and interfaces of these materials. Nevertheless, it is imperative to understand these mechanisms and interfaces, and their influence on the performance of ion conductors, in order to design next-generation materials and devices, as well as improving existing technologies. In this presentation, I will discuss how atomic-scale simulations can help us in the understanding, design and improvement of next-generation solid electrolyte materials for solid-state batteries. In particular, I will present some of our recent work on the influence of grain boundaries on ion transport in different solid electrolyte families and how we can discriminate between the complex correlation factors that determine the characteristics of ion transport. The importance of the synergy between modelling and experiment in the development of new energy materials will also be disseminated.

A3.3

Synthesis of Diverse Nanocomposite Materials for Lithium Battery and Water Electrolysis Applications

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Addressing challenges surrounding lithium (Li) metal anodes requires innovative approaches in material design. While non-Li-alloying materials offer structural stability during cycling by minimizing lattice distortions, their efficacy is hampered by low lithiophilicity and sluggish mass transport kinetics. To tackle these issues, we propose a synergistic strategy aimed at enhancing intrinsic lithiophilicity and mass transport kinetics of non-Li-alloying nucleation sites, showcasing remarkable effectiveness.[1] We fabricate two distinct carbon fiber (CF) hosts, one coated with non-Li-alloying nanosheets and the other incorporating an oxygen-enriched carbon filler (OCF) to serve as a lithiophilicity and mass transport enhancer. Through comprehensive physiochemical evaluations, including advanced techniques such as 3D tomography and location-dependent electron energy loss spectroscopy, we elucidate the intricate heterostructure of OCF-DSC@CF, delineating the distinct roles of each constituent. The incorporation of OCF significantly enhances lithiophilicity and mass transport kinetics, as confirmed by theoretical and electrochemical analyses. Furthermore, OCF-DSC@CF fosters the development of a multifunctional solid electrolyte interphase (SEI) enriched with LiF and LiCx, demonstrating balanced electrical resistivity and ionic conductivity. This study not only opens up new avenues for designing 3D hosts across various electrochemical systems but also underscores the importance of advanced material characterization techniques and systematic electrochemical analyses in gaining deeper insights into material performance.

Water electrolysis has garnered significant attention in research circles due to its potential applications in sewage disposal, microorganism treatment, and large-scale hydrogen production via direct electrolysis. In this presentation, I will also delve into our recent advancements in the synthesis of diverse electrocatalysts tailored for water electrolysis. Our focus lies in exploring cost-effective and efficient electrocatalysts for this process, particularly centering on harnessing the capabilities of iron, one of the most abundant transition metals on Earth. We employ three key strategies—morphology control, secondary metal integration, and nitrogen doping—to fully unleash the potential of iron in water electrolysis.

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A4.1

Droplet-based Nanoreactors for Catalysis and Nanostructure Fabrications

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Surface nanodroplets are referred to 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 talk, *in situ* formation and assembly of nanostructures in surface nanodroplets. Each droplet served as a nanocompartment to confine the nucleation and growth of nanomaterials as well as a template for nanomaterial assembly.

Here, the controllable generation of flower-shaped surface gold nanostructures (FSGNs) within nanoscale surface droplets is demonstrated as an example.⁴ The morphology and structure of the resulting Au nanostructures are governed by internal convection flows and interfacial energy, modulated by the nanodroplet composition and substrate wettability. The obtained FSGNs are proven to act as versatile scaffolds for the selective generation of Au spiky nanostars. These FSGNs can also be utilized to functionalize nanodroplet-based reactors, boosting the fluorescent intensity of Nile red (NR) fluorophores and decomposing NR via catalytic reaction. Remarkably, with FSGN functionalized droplets smaller than a radius of 500 nm, the decomposition rate of NR can reach ≈ 0.01 s-1. These results highlight the potential of surface nanodroplets as novel miniaturised platforms for nanomaterial synthesis, nanostructure fabrication, and catalytic degradation in nanoscale.

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A4.2

Developing devices and characterisation tools for efficient and stable photoelectrochemical cells based on earth-abundant materials

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Photoelectrochemical cells (PECs) offer a potential pathway towards sustainable fuel production, for example through solar-powered water splitting into oxygen and hydrogen fuel. However, so far high solar-to-fuel generation efficiency (>15%) has only been demonstrated using expensive and scarce inorganic III-V semiconductor photoelectrodes. PECs based on next-generation solution processed semiconductors (e.g. metal-halide perovskites, organics, and metal oxides) are less resource intensive, enable more environmentally friendly fabrication methods and allow greater choice of material properties compared traditional inorganic technology. However, solution-processed PECs fall far short of the necessary combination of efficiency (>15%) and stability (>2 years) for large-scale deployment.

Here, I will first present protected photoanodes based on organic-semiconductor light absorbers and inorganic-carbon protection sheets that can achieve photocurrent close to the theoretical limit fort their bandgap (\sim 1.4 eV) at 1.23V vs RHE, and with multi-day stability under operating conditions. I will further demonstrate that when combined with a second, wide-band, organic semiconductor light absorber, tandem photoelectrochemical cells with unassisted (zero-bias) solar-to-hydrogen efficiency exceeding 5% can be fabricated, amongst the highest reported efficiency for photoelectrochemical devices based on non-toxic and earth-abundant materials.

In the second part, I will present a new photoelectrochemical characterization tool, photo-electrochemical mass spectrometry (PEC-MS), that enables, for the first time, the real-time detection of multiple photoelectrochemical reaction products with pico.mol.s⁻¹ sensitivity. I will demonstrate how this tool can be used to gain novel insight into the photoelectrochemical and photocatalytic reaction and loss pathways in existing materials (hematite, bismuth vanadate), and aid the development of better photoelectrochemical and photocatalytic devices.
A5.1

The application of CaO/CuO materials in different integrated Calcium and chemical looping cycles

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In integrated calcium and chemical looping applications, maintaining high CO₂ uptake is crucial. This study examined three materials with a fixed Cu/Ca ratio of 1.6 to understand the factors influencing CO₂ uptake. Testing was conducted over 50 cycles in two looping applications: reduction-carbonation-oxidation for blast furnace gas (BFG) cycle, and carbonation-reduction-oxidation for flue gas (FG) cycle. Multi-grain precipitate material (MGP) consistently maintained its phase distribution, i.e. a combination of mixed Ca-Cu-O phases and separate phases of CaO and CuO, throughout both cycling. MGP showed a peak in CO₂ uptake in initial BFG cycles before stabilising, while exhibited stable CO₂ uptake in FG cycling. The other two materials, MM1 and MM2, prepared through mixing and calcination at different temperatures (800°C and 950°C respectively), displayed mixed Ca-Cu-O and CuO phases, with no distinct CaO phase. MM1 had a more porous surface, whereas MM2, calcined at 950°C, showed sintering. During both cycling, the phases in MM1 and MM2 evolved towards those in MGP. In BFG cycling, MM1 showed slightly higher stabilised CO₂ uptake compared to MM2, likely due to its more porous surface. In FG cycling, MM1 initially experienced a decrease in CO2 uptake, while MM2 showed an increase. However, after the first 5 cycles, MM1 and MM2 stabilised at similar levels of uptake. Surface morphology appeared to influence CO₂ uptake while not significantly. Additionally, the stabilised levels of CO₂ uptake were less dependent on the initial phase distribution but were governed by the nature of cycling process. BFG cycling gave a much higher uptake.

A5.2

The Role of Electron Microscopy and X-ray Microtomography in Lithium-Ion Materials Characterization

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In contemporary battery research, the key objectives are to enhance production processes, advance existing battery technologies, and create new energy storage solutions that offer high capacity, long lifespan, rapid charging and discharging, safety, and eco-friendliness, supporting a future without fossil fuels. Achieving these goals relies on thorough, multiscale structural and chemical characterization of lithium-ion battery materials.

This presentation underscores the crucial role of advanced microscopy techniques, such as Scanning Electron Microscopy (SEM), Focused Ion Beam-Scanning Electron Microscopy (FIB-SEM), Scanning Transmission Electron Microscopy (STEM), and micro-computed tomography (micro-CT), in characterizing both conventional and next-generation lithium-ion battery materials. SEM delivers detailed images of surface morphology, allowing for the analysis of particle properties, degradation mechanisms, contaminants, and structural integrity. FIB-SEM enhances this analysis with subsurface and three-dimensional imaging, unveiling the internal micro- and nanostructures, solid electrolyte interphase, and phenomena like voids, cracks, and delamination. STEM provides nanoscale compositional characterization of active materials and components, including their surfaces and interfaces. Micro-CT offers non-destructive, three-dimensional imaging of the entire battery cell or module architecture and materials, revealing intricate details.

These techniques empower researchers to optimize battery properties, identify and prevent failures, and develop sustainable energy solutions. They tackle challenges posed by material chemistries and battery processes, guiding advancements in battery design and production.

B1.1

Electrochemical lithium intercalation & exfoliation in 2D TMDs and its in-situ studies

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We developed a lithium ion battery intercalation & exfoliation method with detailed experimental procedures for the mass production of 11 two dimensional TMDs and inorganic nanosheets, such as MoS₂, WS₂, TiS₂, TaS₂, ZrS₂, graphene, h-BN, NbSe₂, WSe₂, Sb₂Se₃ and Bi₂Te₃, among them 3 TMDs achieved mono- or double layer yield > 90%. This method involves the electrochemical intercalation of lithium ions into layered inorganic materials and a mild sonication process. The Li insertion can be monitored and finely controlled in the battery testing system, so that the galvanostatic discharge process is stopped at a proper Li content to avoid decomposition of the intercalated compounds. The intercalation strategy can also be used to tune 2D TMDs' physical and chemical properties for various applications. For example, we developed a one-step covalent functionalization method on MoS₂ nanosheets for membrane fabrication, which exhibited excellent water desalination performance. For lithium intercalation mechanism, the stateof-the-art In-Situ Liquid Phase TEM is an ideal technique for identifying the phase changes during intercalation process. With self-designed electrochemical liquid cell utilized, we can directly vapture the dynamic electrochemical lithiation and delithiation of electrode in a commercial LiPF6/EC/DEC electrolyte, such as LiF nanocrystal formation, lithium metal dendritic growth, electrolyte decomposition, and solid-electrolyte interface (SEI) formation. Combining with other in-situ techniques, such as in-situ XAS, XRD and Raman, etc, the underlying lithium intercalation mechanism in TMDs were further investigated, which render us a comprehensive understanding of the intrinsic correlation between the intercalation process and TMDs layered structures.



Figure 1 (A) Lithium Ion Intercalation Strategy to prepare 2D transition metal dichalcogenide (TMD) nanosheets; (B) In-Situ Liquid Phase TEM to probe cathode-electrolyte interphase.

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B1.2

Spatially resolved in operando temperature sensing in electrochemical devices

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Temperature plays a crucial role in the operation of electrochemical devices, serving as both an indicator of device efficiency and stability. However, the complex material architecture within the device, coupled with local variations in electrochemical activity, leads to a time-dependent and spatially varying temperature at the nanoscale. This nanoscale temperature can significantly differ from the average temperature measured at the macroscale. Unfortunately, obtaining information on the spatially resolved temperature evolution is challenging due to the lack of non-invasive and accurate nano-thermometry methods that meet the requirements for sensitivity, spatial resolution, and temporal resolution within the reactive chemical environment of a functional device. In this presentation, I will discuss our recent progress in sensing schemes that utilize ND quantum sensors to monitor the spatially resolved temperature evolution in operational electrochemical devices, such as battery cells or electrolyzers. By employing nanodiamond (ND) sensors, our measurements have revealed that the local temperature within the working device is considerably higher than the spatially averaged temperature measured using conventional methods. Furthermore, we have observed that the spatial temperature distribution evolves in conjunction with the respective electrochemical processes. This work is carried out in collaboration with Renbao Liu, Wenghang Leung, Ruqiang Dou, Zan Li, Hui Wang, Yi Xie, Yao Gao, Ying Wang, and Chunyi Zhi. The authors acknowledge funding support from RGC CRF C4004-23G.

B1.3

Fuelling a Sustainable Future: Strained Hydrocarbons for High-Energy-Density Aviation Fuel Screened using ML and DFT Calculations

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Aviation industry is the biggest air polluter and aviation fuel is the blood of aircraft. While advancements toward cleaner energy sources like hydrogen or batteries remain on the horizon, sustainable aviation fuel (SAF) emerges as a vital interim solution for the coming decades [1].

The composition of aviation fuels such as Jet A/A-1, JP-5, and JP-8 are very similar, which consist predominantly of C9–C16 hydrocarbons that are a combination of n-paraffins, isoparaffins, naphthenes, and aromatics. SAF, predominantly composed of hydrocarbons derived from the Power to Liquid (PtL) pathway (i.e., hydrogen obtained through water splitting and carbon recycled from CO₂) represents a near-carbon-neutral alternative [1]. High energy density (HED) aviation fuels are dominated by multicyclic strained hydrocarbons, particular polycycloalkanes, however, the precise connection between their quantitative structure and property relationship (QSPR) remains less understood. The present study uses a known group of high energy density (HED) hydrocarbons to train machine learning (ML) models, which are applied to select the structures of strained cyclic hydrocarbons with required net heat of combustion (NHOC) and density for aviation fuel applications. Quantum mechanical based density functional theory (DFT) calculations were applied to selected structures of hydrocarbons. Preliminary results are presented.



Figure 1. (a) Impact of NC (Number of carbons) to net heat of combustion (NHOC). (b) DFT calculated 13C-NMR chemical shift of norbornyl derivatives.

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B2.1

Electrolyte Engineering for rechargeable aqueous Zn-ion batteries

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In consideration of increasingly severe carbon emission issues and rigid stipulations for low-carbon society objectives, current electrochemical energy storage systems require a radical upgrade to meet various application demands from end users. Aqueous zinc ion batteries (AZIBs) provide sustainable routes to gridscale energy storage systems because of their cost and safety advantages by using mild aqueous electrolytes and abundant metallic zinc anodes. Besides, owing to the distinctive merits such as relatively high ionic conductivity, environmental benignity, low risks of flammability and considerable energy density of AZIBs compared with conventional Li-ion batteries, AZIBs are intensively investigated to unleash the potential for practical applications. However, the development of rechargeable AZIBs is plagued by poor reversibility due to a series of intrinsic issues, such as hydrogen evolution and Zn dendrite formation. Significantly, the advances in materials discovery and innovation in device configuration have improved the performance of AZIBs in all aspects, including durability, operating voltage range, energy/power density, and economic availability. Different electrolyte components are investigated intensively to suppress the side reaction on the Zn anodes. However, further improvements are needed, especially for realizing the requirement for high energy density and high stability scenarios. The recent progress of AZIBs technology, such as facile electrolyte components and additives for aqueous AZIBs will be discussed in this talk.

B3.1

Lignocellulosic biomass-derived functional materials

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An industrial production of biomaterials and bioethanol from lignocelluloses such as corn cob and other cereal straws by a combination of hydrothermal pre-treatment and alkali post-treatment based on a biorefinery scenario have being performed at Shandong Longlive Bio-Technology Co., Ltd, since 2011 in China, in which 30 thousands tonnes of bioethanol, 6 thousands tonnes of xylo-oligosaccharides (XO) and 10 thousands tonnes of xylitol with a purity of more than 97%, 300 tonnes of arabiose with a purity of more than 98.5%, and 10 thousands tonnes of lignin with a purity of more than 94% have being produced from 200 thousands of corn cob per year. The XO can be used as food additives and nutraceuticals, which have favorable technological properties and cause prebiotic effects derived from their ability to modulate the intestinal function.

In addition, over 50 million tons of lignins are produced as a byproduct from the paper manufacturing and biorefinery industries every year. Owing to its aromatic nature and abundant resources, lignin is therefore widely used to serve as precursors and fillers to prepare biodegradable polymers and improve antioxidation or light stability of bio-based composites. In this report, the industrial lignins recovered as a by-product from the bioethanol production and papermaking process, were activated under alkaline conditions and then used to produce lignin-phenol-formaldehyde (LPF) adhesives with a yield of about 60 thousand tons per year for partially replacing the expensive phenols (50%) in the commercial production of biocomposite boards for construction and furniture in China today. Another industrial utilization of the by-products of lignins as rubbish bags in shanghai city and agricultural mulching films on farms will be reported. Furthermore, the modified lignin as a protective film to control lithium growth for high-performance lithium-metal batteries will be also reported.

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BIO



Professor Run-Cang Sun, ligniocellulosic chemist, got bachelor degree at the chemistry department, North-western University, Xian, China in 1982 and PhD degree in 1996 at The BioComposites Centre, University of Wales, Bangor, UK. He worked at University of Wales, South China University of Technology and Beijing Forestry University. He was the director of State Key Laboratory of Pulp and Paper Engineering (2008.8-2015.5, part time) and Dean of College of Materials Science and Technology (2011.10-2014.9). Since March 2019 Prof. Sun has being working at Liaoning Key Laboratory of Lignocellulose Chemistry and BioMaterials as a director, Dalian Polytechnic

University, Dalian, China. He has being focused on biomaterials, biofuels, and chemicals from lignocellulose. He has published 995 SCI papers in peer reviewed international journals, which have been totally cited over 65,000 citations (his Google Scholar h-index of 126). As invited author, he also authored 36 book chapters regarding utilization of lignocelluloses for biomaterials. He has awarded 164 patents for inventions. He is the recipient of the ACS Cell Division Anselme Payen Award 2020. He has ranked No. 1904 in the ranking of The Top 100,000 Scientists in the World and 185 in the world ranking of Top 1000 Scientists in the area of Chemistry (2022).

Prof. Sun is a Fellow of The Royal Society of Chemistry, UK in 2003 and an Editor-in-Chief of Industrial Crops and Products, Associate Editor of Carbohydrate Polymers, Frontiers In Energy Research and Journal of Biobased Materials and Bioenergy. He is also a member of editorial board in ChemSusChem, Journal of Agricultural and Food Chemistry, International Journal of Cellulose Chemistry and Technology, Bioresources and Bioprocess, Molecules, EcoMat, etc.

B3.2

New Insights into the Cation Disordered Rocksalt Chemistry via Pair Distribution Function

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Cation disordered rocksalt (DRX) materials are promising electrode alternatives for the next-generation battery technology due to their superior performances concerning capacity and rate capability. These materials are usually prepared via heat treatment or mechanochemical synthesis. Recently, several cation DRX oxides with desirable cycling behaviours have been prepared through electrochemical lithiation of a series of binary metal oxides that have a non-fcc oxygen sublattice. Capitalizing on these findings, we strategically investigated several metal oxides with unique oxygen structures and employed pair distribution function (PDF) for phase characterization. Through the use of a big data approach via the Metropolis non-negative matrix factorization (MMF)⁽¹⁾ for a robust phase deconvolution against the PDF data, cation DRX intermediates were identified in these oxides upon electrochemical lithiation. Jointly with the earlier reports, these new findings constitute empirical evidence pointing to a general principle that underpins the electrochemical DRX transformation, opening up new opportunities for the development of higher energy density batteries.⁽²⁾

In addition, despite the nomenclature "cation-disordered", some recent experimental studies have reported observations of cation short-range ordering (SRO) in these DRX oxides, whose (local) structure type, as well as the degree of (dis)order, was found to show a significant impact on the local mobility of Li+ and its percolation (i.e. long-range diffusion). A clear understanding of these materials' cation SRO is therefore critical to rationalize their electrochemical properties. Therefore, a new methodology will be presented to access the cation SROs by decomposing their PDF data into a set of basis PDFs pre-determined via the MMF analysis. As a proof of concept, we show that these basis PDFs, underpinned by structure modelling, point to specific SRO types that subsequently could enable structure identification and quantification of their presence in the DRX materials⁽³⁾.

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B3.3

Phosphorus-Based Anode Materials for Fast-Charge Li-ion Batteries

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Researchers have spent years improving the capacity of electrode materials to boost the energy density of Li-ion batteries and recently have paid increasing attention to reducing the charging time. The Advanced Battery Consortium targets batteries of energy density >275 Wh/kg or 550 Wh/L and can recover 80% of its nominal energy in 15 minutes. At the cell level, however, the charging rate (power density) of the batteries is limited by the electrochemical properties of the anode materials, which, when recharging at a high rate, tends to precipitate lithium metals due to the drop of the anode potential below Li/Li⁺ and the relatively faster capacity decay than the cathode. An anode material that holds a large theoretical capacity and promising electronic and ionic conductivities, as well as moderate electrochemical potential, is demanded to tackle the issues in anode for Li-ion batteries when fast recharging. Phosphorus-based anode materials have been recently identified as a promising choice for Li-ion batteries where fast recharge capability is required, but a series of issues still need to be considered. We will introduce our recent progress in phosphorus/carbon composites by tailoring the interface structure to boost the Li-ion transport and structure stability for high-rate, high-capacity Li-ion storage.^[1-5]

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B4.1

Atomic-scale design of anode materials for rechargeable batteries: from carbons to metals

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The development of high-performance anode materials for rechargeable batteries is crucial for the green energy evolution. In this talk, I will introduce our endeavor in designing different types of anode materials using density functional theory (DFT) and molecular dynamics (MD) simulations, combined with experimental efforts [1].

Carbon materials (graphene, graphite, and hard carbons) are widely used as anode materials for Li-ion, Naion, and K-ion batteries, due to their abundance, stability, and low-cost advantages. We have used DFT and MD simulations of Li, Na, and K on different carbon structures found in various carbon materials to investigate their effects on the metal incorporation and migration mechanisms in relation to battery storage capacity and charge/discharge cycling ability [2-5]. These atomic-scale understandings have led to a revised mechanistic model for Na insertion in hard carbons for NIBs [6], and could improve design of carbon materials for rechargeable batteries. Our work on conversion-type and alloying-type anode materials will also be discussed, using examples of Bi₂S₃ for Li-ion batteries [7], and Bi for K-ion batteries [8].

Metal anodes are ideal for achieving high energy density rechargeable batteries, due to their high storage capacities and low electrochemical potentials. I will introduce our collaborative efforts in developing solutions electrolyte (e.g., electrolyte additives [9], and ion implantation of solid electrolyte [10]) for supressing the Li dendrite growth, for enhancing the stability of Li metal and cycle life of batteries. Finally, I will introduce our ongoing work on metal anodes including using DFT simulations to understand the Li nucleation behaviour on the pristine and defected Li (100) surfaces, and to screen interlayer materials that can enable the stable deposition/stripping process of Li during the operation of zero-excess solid-state Li/Na batteries using a modelling framework combining DFT calculations and molecular dynamics (MD) simulations with trained machine learning (ML) potentials.

Acknowledgement:

We would like to acknowledge the funding support from UKRI EPSRC (EP/R021554/1), the Faraday Institution for *LiSTAR - The Lithium-Sulfur Technology Accelerator* programme (grant number FIRG058), and Horizon Europe for the OPERA project (grant number 101103834). We would also like to thank the UK Materials and Molecular Modelling Hub for computational resources, which is partially funded by EPSRC (EP/T022213 and EP/W032260).

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B4.2

Repair and reuse of spent lithium battery electrode materials

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With the popularity of new energy vehicles and various electronic devices, the use of lithiumion batteries (LIBs) has shown explosive growth, which has resulted in a large number of spent LIBs. Spent LIBs contain a large amount of metal resources, and improper disposal will not only cause waste of resources, but also have potential environmental risks. The existing commercial recycling methods are mainly pyrometallurgy and hydrometallurgy recycling methods, both of which require re-extraction from the electrode material after destroying them to the atomic level for the preparation of new electrode materials, which is a long process with high cost, and involves the application of extreme conditions such as high temperature and strong acid, with inferior economic and environmental benefits. It is a major challenge in the field of battery recycling to develop innovative and clean recycling methods, to simplify the recycling process and to develop ways to reuse the recovered products. In view of the challenge of existing recycling methods, the reporters proposed the idea of direct recycling of electrode materials at the molecular scale, and designed innovative recycling methods such as direct repair of degraded lithium cobalt oxides with deep eutectic solvent (DES), repair of Ni-Mn-Co ternary (NCM) cathode with high failure degree by low temperature molten salt, and thermal regeneration of degraded lithium iron phosphate (LFP) with multifunctional solvent; and closed-loop design of the direct recycling process. In addition, we propose a high-value utilization path for the conversion of degraded electrode materials to high-performance electrode materials and nano-catalysts. It greatly simplifies the recycling process, avoids the use of extreme conditions, and provides a new technical system and theoretical guidance for battery recycling research and industry.

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C1.1

Standalone stretchable device platform for biomedicine

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Conventional electronics today form on the planar surfaces of brittle wafer substrates and are not compatible with 3D deformable surfaces. As a result, stretchable electronic devices have been developed for continuous health monitoring. Practical applications of the next-generation stretchable electronics hinge on the integration of stretchable sustained power supplies with highly sensitive on-skin sensors and wireless transmission modules. This talk presents the challenges, design strategies, and novel fabrication processes behind a potential standalone stretchable device platform that (a) integrates with 3D curvilinear dynamically changing surfaces, and (b) dissolves completely after its effective operation. The resulting device platform creates application opportunities in fundamental biomedical research, disease diagnostic confirmation, healthy aging, human-machine interface, and smart Internet of Things.

Biography:

Prof. Huanyu "Larry" Cheng is the James L. Henderson, Jr. Memorial Associate Professor of Engineering Science and Mechanics at Penn State University. His research group focuses on the design, fabrication, and application of the standalone stretchable device platform. Larry has co-authored more than 150 publications with total citations >20,000 according to Google Scholar. His work has been recognized through the reception of numerous awards, including the 2024 Robert and Maude Gledden Visiting Fellowship at the University of Western Australia, Highly Cited Researcher in the field of Cross-Field in 2023, 2023 Emerging Investigator for Journal of Materials Chemistry C and Nanoscale, Humboldt Research Fellowship for Experienced Researchers, 2022 Minerals, Metals & Materials Society (TMS) Functional Materials Division (FMD) Young Leaders Professional Development Award, 2021 NIH Trailblazer Award, MIT Technology Review Innovators Under 35 (TR35 China) in 2021, 2021 Scialog Fellow in Advancing BioImaging, 2021 Frontiers of Materials Award from TMS, Forbes 30 Under 30 in 2017, among others. He also serves as the associate editor for 7 journals and reviewer for > 270 journals.

C1.2

Novel fibre synthesis from textile waste materials

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Textile industry is a major plastic consumer and plastic waste generator. Synthetic polymers in textile waste are a major contributor to global plastic waste crisis. In 2017, 438 M tonnes of plastic were produced worldwide; 62 M tonnes were used in the textile industry and 158 M tonnes in plastic packaging. While plastic packaging has attracted attention and concern for some time, textile waste has only become prominent recently, in part because recycling textile waste is a highly challenging task. In the UK, over 1 M tonnes of textile waste are generated annually. Recycle textile waste is an urgent request for the waste management and a desire demand for circulate economy.

In this report, a biorefining strategy for the recycle of textile waste will be introduced. Fungal fermentation using textile waste was carried out for the production of cellulase, which is then used for the degradation of textile waste. The degraded textile waste was subject to separation to recover recycled PET fibre. The impact of cellulase loading on the separation cellulose from PET fibre was investigated, and its impact on the recycled PET fibre physiochemical properties have been tested as well. Then, the recycled PET fibre was used for the spinning of new fibre via melt spinning method.

C1.3

Atomic Design of Transition Metal Catalysts for High-Efficient Hydrogen Production

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With the highest gravimetric energy density and water being the only combustion product, hydrogen is one of the most attractive fuels for global energy sustainability and a future low-carbon economy. Transition metal materials exhibit superior catalytic performances toward hydrogen production and utilization, and developing cost-effective, highly active, and stable catalysts will significantly advance the hydrogen economy. The atomic design of transition metal-based materials provides a promising approach to reducing metal usage and improving their catalytic performance. Since the majority of catalytic reactions proceed at the surface and/or interface sites, atomically engineering these active sites is essential to design high-efficient and low-cost catalysts, which can also contribute to investigating the relationship between material, structure, and performance.

Herein, by atomically engineering transition metal-based catalysts on their surface and/or interface structures, we optimized both the cathodic and anodic reactions towards water splitting to produce hydrogen and improved the catalytic performance towards various selective hydrogenation reactions. Specifically, we designed the ultrathin two-dimensional Pd nanomesh with abundant surface and interface sites, promoting the accurate deposition of the ultrasmall Pt nanoparticles on these active sites, and thereby significantly enhancing the catalytic activity and durability of hydrogen evolution reaction (HER). We then systematically investigated the enhancement of spin-polarized oxygen evolution reaction (OER) under the magnetic field by atomically designing the magnetic spinel catalysts, and built a magnetism/OER activity model that provides new design principles for active OER catalysts. Furthermore, by atomically regulating the size and atomic arrangement of precious metals, we synthesized the monolayer and atomically dispersed Ru, as well as the heterophase of Rh, which significantly improved the catalytic performances of various selective hydrogenation reactions.

C2.1 Muhammad Wakil Shahzad

C3.1

Towards self-powered touch/force/motion sensing through coplanar reverse electrowetting-on-dielectric energy harvester

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A highly energy efficient and sensitive touch/force/motion sensing mechanism through liquid deformation induced electrical signal has been proposed and demonstrated, with great potential to be self-powered Compared to conventional capacitive sensors, liquid-electric energy through design optimization. generation micro-transducers such as ionovoltaics [1] and hydrovoltaic [2] and reverse electrowetting-ondielectric (REWOD) [3-6] have provided an opportunity to make sensing more energy efficient or even self-powered. Previous REWOD studies have been using a two-plate electrode structure while this study frees up the topside space by using a single plate coplanar structure (Fig. 1a). The allows for better versatility in materials and applications, for example, to have a flexible top structure to deform the liquid in response to a versatile range of mechanical inputs such as touch, force, and motion (Fig. 1b) [7]. Low electric noise electric-shake table with vibration amplitude in mm and sub-mm scales were established to characterise the motion sensing against key parameters such as energy harvesting/sensing electrode (EHE) and counter electrode (CE) area ratios (Fig. 1c), dielectric constant value and layer thicknesses, droplet sizes, vibration frequency and amplitude etc. Next, input bias REWOD voltage values and output signal amplitude levels have been comparatively studied, giving hints to potential "bias-voltage-free" selfpowered sensing possibilities.



Figure 1. (a) Schematics show the comparison between conventional REWOD (top) and coplanar configuration REWOD (bottom). (b) The flexibility in coplanar REWOD sensor design where droplet deformation could be induced by various top structure design. (c) Design parameters considerations such as dielectrics (e.g. Ta2O5) and EHE:CE area ratios.

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C3.2

Shielding effect enables ultrafast ion transfer through nanoporous membrane for highly energy-efficient electrodialysis

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A key to sustainable management of hypersaline organic-rich wastewaters is to precisely fractionate organic components and inorganic salts (NaCl) as individual resources. Conventional nanofiltration and electrodialysis processes suffer from membrane fouling and compromise the fractionation efficacy. Here, we develop a thin-film composite nanoporous membrane (NPM) via co-deposition of dopamine and polyethyleneimine as a highly anion-conducting membrane (ACM). Experimental results and molecular dynamics simulations show that co-deposition of dopamine and polyethyleneimine effectively tailors the membrane surface properties, intensifying the charge shielding effect and enabling ultrafast anion transfer for highly efficient electrodialysis. The resulting NPM exhibits unprecedented electrodialytic fractionation of organics and NaCl (>99.3% desalination efficiency; >99.1% organics recovery) with negligible membrane fouling, dramatically outperforming state-of-the-art anion exchange membranes. Our study sheds light on facile design of high-performance ACMs and associated new mass transport mechanisms in electrodialytic separation, paving the way for sustainable management of complex waste streams.



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C3.3

Biodegradation of Nigerian crude oil and the quantification of the key functional genes in a microcosms study with some selected bacterial species

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GC-MS and qPCR have been used to facilitate the profiling of metabolites from a wide range of oil materials leading to the wide coverage of comprehensive central pathways involving primary metabolism and the quantification of functional genes responsible for the biodegradation of crude oil components. Therefore, the present study aimed to explore the ability of *Bacillus endphyticus* and *Pseudomonas lurida* for the biodegradation of crude oil. Microcosms study was also conducted for the degradation of crude oil using Pseudomonas aeruginosa and Pseudomonas lurida. The GC-MS analysis showed an extensive elimination of hydrocarbons of mostly low and medium-chain hydrocarbons by these novel B. endophyticus and P. lurida as well as P. aeruginosa and B. subtilis. The qPCR analysis of the functional genes showed a substantially higher relative fold expression of benzoate monooxygenase gene (Ben) of 2.1x1014 fold after the first week (T1) in a microcosm study with P. lurida. Hence, this could indicate an immediate activation of this gene following the experiment set up. However, low relative gene fold of 60.91 for cat23 was observed in the same microcosm. In the same vein, the relative fold expression of 2156.87 was detected for alkB gene from the microcosms with P. aeruginosa. Thus, this is substantially higher than the expression for *cat23* gene and greatly lower than the *Ben* gene. The overall results of this study could evidently prove the environmental application of this novel bacterial species -B. endophyticus and P. lurida for the management of crude oil polluted environments and the overall finding from this study could be utilised as a tool to design an engineered bioremediation process to address the long devastating crude oil pollution across the Niger Delta and beyond.

C4.1

Realistic evaluation of prototypical porous materials for carbon capture

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Carbon capture, utilization, and storage (CCUS) is an attractive approach to help decarbonization from point sources, like energy supply and other industries, as well as for pulling CO_2 out of the atmosphere (i.e., direct air capture, DAC). Among several approaches at differing technology readiness levels, solid sorbents are promising as they generally combine high uptakes and selectivity with milder regeneration energies.¹

Adsorption screening and testing of promising materials are often performed using pure component or point uptake experiments, which only give information about adsorption capacity and ideal selectivity. At realistic process conditions, competitors such as moisture and temperature have a large effect on the uptake of CO_2 , wherein the presence of water could either increase CO_2 capacity, compete for the same adsorption sites, or even induce material collapse. The kinetics on the other hand is another important factor for an effective separation.²



Figure 1. (a, left) Apparent CO₂ uptake decrease by 5% RH in Zeolite 13X and (b, right) detail of the sorption kinetics of both components highlighting replacement effects.

In this work, several porous materials including zeolites, MOFs, and functionalized resins are screened in realistic conditions for CO_2 capture using advanced dynamic gravimetric sorption and breakthrough methods. The tests were conducted under varied conditions, e.g., different CO_2 concentrations and relative humidity. The results showed that humidity is the key factor affecting the CO_2 capture efficiency. This study provides a reference for screening the effective sorbents for carbon capture.

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D1.1

Stability of perovskite solar cells – effect of perovskite composition and deposition conditions

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Perovskite solar cells (PSCs) have attracted significant attention due to their high efficiency, but their operational stability still needs significant improvement. Different perovskite layer compositions have been reported in the literature,^[1-3] but systematic comparisons of high performance perovskite compositions in terms of stability have been scarce. Here we compare commonly used triple cation CsFAMA perovskite (13% Br, MA denotes methylammonium, FA denotes formamidinium)^[1] to low Br content perovskite (2% Br)^[2] and MA-free perovskite.^[3] In all three cases, cells with efficiency exceeding 20% can be obtained for optimized deposition conditions. However, significant differences in stability and processing window can be observed for different perovskite compositions. While it would be expected that eliminating MA as the least stable cation and reducing Br content to prevent photoinduced segregation would result in improved stability, this is not the case. MA-containing low-Br perovskite^[2] is extremely sensitive to processing conditions, in particular the solution temperature/ambient temperature of the glove box. This perovskite composition guickly degrades upon exposure to atmosphere and under illumination. MA-free perovskite^[3] exhibits considerably better stability in ambient compared to low-Br^[2] perovskite, but devices based on CsFAMA-based perovskites exhibit overall best stability and lower sensitivity to processing conditions among three different perovskite compositions considered. The effect of the perovskite composition on the film and device stability under different stressors (light, oxygen, humidity, bias) is discussed in detail.

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D1.2

Functional Hydrogels and Bioelectronic Interfacing

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Hydrogels are emerged as one of the most idealist material systems to bridge the interface between the biological tissues and electronics, in light of their similarity in composition and structure. However, it is highly challenge to form seamless interface between the hydrogel and biological tissues, due to the presence of free water at the interface. In order to address those challenges in the tissue-electronic biointerfacing technology, such as residues of small molecules, uncontrollable swelling of hydrogel materials, and interfacial failure under extreme conditions, we have designed and fabricated a series of functional hydrogels with unprecedented properties and functions for tissue-electronic biointerfacing.



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D1.3

Interfacial Charge Transport Regulation in Perovskite Solar Cells

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Organic-inorganic hybrid perovskite materials possess excellent optoelectronic properties, leading to the rapid development of perovskite solar cells (PSCs) in recent years. Interfacical charge transport is one of the key factors determining the performance of PSCs. We have developed a series of strategies to regulate interfacial charge transport, effectively improving the performance of PSCs. Specifically, based on the strong electron affinity, high electron mobility, and low recombination energy of fullerene, fullerene-based functional materials have been widely applied in PSCs as electron transport layers, cathode interface layers, or defect passivation agents. This talk will introduce the work of our group in recent years on the development of novel fullerene derivatives and their application as additives in the electron transport layer or perovskite active layer of PSCs.

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D2.1

Material and Device Design for Multijunction Perovskite Solar Cells

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Metal halide perovskite solar cells have become a viable option for future renewable energy. Record single and tandem junction all-perovskite solar cells already provide power efficiencies of over ~26% and ~29%, respectively. A next target in photovoltaic energy conversion can possibly be met by developing perovskite triple or even quadruple junction solar cells. While these hold a promise to afford higher efficiencies, they require developing stable perovskite sub-cells with bandgaps in the range of 1.8 to 2.3 eV, i.e., a range that has not received much attention so far. These wide-bandgap perovskites often suffer from more pronounced voltage losses due to non-radiative bulk and interfacial charge recombination. In developing new perovskite sub-cells, photocurrent spectroscopy and absolute photoluminescence spectroscopy are used in combination with bulk and interface passivation strategies to identify and eliminate these losses. This has enabled to reduce the voltage deficit over a wide range of bandgaps. Guided by optical modelling, monolithic multi-junction solar cells have been fabricated by stacking two and three different bandgap perovskite sub-cells in series using recombination junctions that have been designed to provide near-zero electrical and optical losses. Collectively, these strategies enable monolithic tandem and triple junction solar cells with a power-conversion efficiency of over 26%. Photoluminescence of individual sub-cells provides information on the internal voltage in each absorber layer and offers a detailed understanding of the performance-limiting components in the tandem solar cell following prolonged continuous operation.

D3.1

Electricity-free heating and cooling strategies for water and energy sustainability

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Addressing global challenges necessitates advancements in energy and water sustainability. Direct solar desalination, for instance, holds immense promise for alleviating the worldwide freshwater crisis. This presentation will delve into practical considerations for developing solar heating and radiative cooling applications that promote water and energy sustainability. Specifically, I will discuss our recent advancements, spanning manufacturing to application development. We will begin by exploring our research efforts to create low-cost solar-driven evaporation architectures using photothermal materials and systems [1-3]. Additionally, we will discuss the potential applications of these architectures for zero-liquiddischarge water treatment using evaporation ponds.

However, if the evaporated moisture cannot be collected, it merely contributes to atmospheric pollution. As the entropy sink, the cold source plays a crucial role in completing the thermodynamic cycle of all heatproducing technologies. The unique challenge lies in obtaining coldness from renewable and sustainable sources.

In the second part of this presentation, we will discuss our recent efforts on radiative cooling in water and energy sustainability [5-9]. Specifically, we will examine the potential of passive cooling technology to recycle atmospheric water. We will also highlight potential pitfalls to avoid in radiative cooling reporting, as summarized in our recent work [10].

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D3.2

Active layer morphology of organic and perovskite photovoltaics – a study based on grazing-incidence X-ray and neutron scattering

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Nowadays, solar industry becomes the fastest growing industry due to the rising demands to solve the energy crisis and environmental problems. Third-generation solar cells, especially organic and perovskite solar cells are all relying on a semiconducting thin-film active layer to harvest the solar energy. The bulk morphology of the active layer in terms of crystal structure, orientation and nanophase separation behaviors is known to be critical to the organic solar cell device performance. Here, we will present our recent studies on the process-structure-device correlation of organic and perovskite solar cells. In these studies, state-of-art grazing incidence scattering techniques using X-rays and neutrons were employed for various purposes, such as grazing incidence wide-angle/small-angle X-ray scattering (GIWAXS/GISAXS), grazing incidence transmission small-angle X-ray scattering (GTSAXS), grazing incidence matter physics studies. By modifying the wavelength of the probing beam and the experimental geometry, a variety of sample types, such as solutions, powders, surfaces and thin films, can be studied, covering wide length scales as well as versatile dynamic and kinetic behaviors.

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D3.3

Engineering Materials and Interfaces for Perovskite Solar Cells and Modules

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Materials, interfaces and active layer crystallization are critical to the functioning of perovskite optoelectronic devices towards applications. In this presentation, I will update our recent work on the development of high-efficiency and high-stability perovskite solar cells and modules. Carbon-based perovskite solar cells show great potential owing to their low- cost production and superior stability in ambient air. However, scaling them up to utility level carbon-based solar modules hinges on reliable deposition of uniform defect-free perovskite films over large areas, which is an unsettled but urgent issue. Over the past few years, we have developed a set of technologies of soft-assembly full-printing carbon-based solar modules. all of the functional layers of the module are printed through a simple and high-speed (300 cm min⁻¹) blade coating strategy in ambient atmosphere. Long-chain surfactant molecules are introduced into perovskite film construction, crystallization kinetics modulation and defect passivation, leading to power conversion efficiencies of >20% for 100 cm² modules and a high stability. This advance marks a significant step toward the commercialization of all-printable carbon-based perovskite solar modules. The prospects and challenges of the solar module development will also be discussed.

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D4.1

Constructing efficient and stable formamidinium-based perovskite photovoltaics

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Perovskite materials, most notably organo-lead iodide species, have recently demonstrated great potential in future high-performance photovoltaics. Formamidinium lead iodide perovskite (FAPbI₃) features desirable bandgap and thermal resistance, and has thus emerged as the most promising candidate among the perovskite family for highly efficient photovoltaic devices. However, the photoactive black-phase FAPbI₃ is not energetically favorable at room temperature. Polytype formation and other intermediate non-photoactive phases can readily occur, which undermines the photovoltaic performance. Through multimodal in-situ monitoring of the perovskite crystallization process, we found an oriented nucleation mechanism that acted as the key to avoid undesirable phases. This concept was applicable to improving the photovoltaic device performance under different film-processing scenarios. In this talk, I will present our recent progress on improving the stablity and efficiency of FA-based perovskites, and the potential of the commercialization will be discussed.

Pengju Shi, Yong Ding, Bin Ding, Qiyu Xing, Tim Kodalle, Carolin M Sutter-Fella, Ilhan Yavuz, Canglang Yao, Wei Fan, Jiazhe Xu, Yuan Tian, Danyu Gu, Ke Zhao, Shaun Tan, Xu Zhang, Libing Yao, Paul J Dyson, Jonathan L Slack, Deren Yang, Jingjing Xue*, Mohammad Khaja Nazeeruddin*, Yang Yang*, **Rui Wang***, *Nature*, 620, 323-327 (2023)

D4.2

Synergy of thermochemical exhaust heat recuperation and ammonia-fired gas turbine for CO₂-free power generation

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Ammonia produced from renewably sourced green hydrogen has recently received international interest for power generation due to its high gravimetric H₂ density, easy-to-store properties and carbon-free structure, resulting in no CO₂ formation. In March 2021, engineers from Japan announced that 40 MW gas turbine fired by 100% ammonia is on the final stage of developing. Moreover, GE and IHI agreed to develop an ammonia fuels roadmap for Asia, with a specific focus on how ammonia fuel could be utilized across existing small and medium-sized gas turbine fleet.

However, when NH_3 is used directly as a gas turbine fuel, the gas turbine suffers from low combustion efficiency due to the low flame speed and long quenching distance of the fuel [1]. The synergy of NH_3 and H_2 is a promising pathway since H_2 can be obtained from thermo-catalytically cracking NH_3 , eliminating the need to store two fuels. In contrast to NH_3 , H_2 is a high flame speed with short quenching distance fuel, resulting in significantly improved and wide-range combustion inside the gas turbines.

This study aims to study the synergy of NH₃ and H₂ (produced from NH₃ decomposition) to trade off the undesirable properties of each fuel and achieve optimal efficiency. Flexible and efficient power generation from NH₃ will promote the utilization of renewable hydrogen while avoiding the H₂-associated drawbacks and hazards, such as high energy losses for its compression or transportation and storage safety risks. The objective and novelty of this study lie in implementing a thermodynamic onboard NH₃ reforming system that utilizes the gas turbine's waste heat and promotes energy conservation [2].

The study of a novel ammonia-fired chemically recuperated gas turbine is divided into three main parts: thermodynamic analysis, chemical kinetics of ammonia decomposition, and combustion of the products of ammonia decomposition.

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E1.1

Self-powered bioelectronics with biomimetic designs and biomechanical energy harvesting

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The use of bioelectronic devices for acquiring biological information and delivering therapeutic interventions relies on direct contact with soft bio-tissues. To achieve long-term stable functions, it is pivotal for such electronics to possess biomimetic form-factors in various aspects and continuous energy supply for achieving long-term compatible and sustainable operations. In this talk, I will first introduce our material and device designs for introducing three highly important biomimetic properties onto transistor-based biosensors—stretchability, tissue-like softness, and bioadhesive properties. Our rationale designs from the material to the device level allow the realization of these properties with state-of-the-art electrical performance. I will also introduce the strategies and advantages of using these new biomimetic properties in bioelectrical and biochemical sensing. In the second part, I will also introduce our work in designing high-efficiency stretchable light-emitting polymers and OLEDs based on thermally activated delayed fluorescence. In the final part, I will introduce our innovative use of polymer chemistry and engineering for achieving stretchable triboelectric nanogenerators that can efficiently harvest energy from human body movements.

E1.2

Polyamide Microfiber /Black Carbon/AgNWs Composite as a High-Performing Sensitive Pressure Sensor

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High-sensitive multifunctional pressure sensors have attracted considerable attention in recent years, for applications in monitoring human motion medical detection, and human–computer interactions. Herein, to improve the sensitivity of the sensor, sea-island polyamide microfiber material was proposed as the flexible mat, and carbon black and silver nanowires as the conductive materials, to prepare the PA/CB/AgNWs flexible pressure-sensitive material by using combined thiol-ene click chemistry and physical blending method. PA/CB/AgNWs composite sensor exhibits a high sensitivity (65.41 kPa⁻¹), quick response (0.10 s) and recovery (0.10 s) times, and a low detection limit range (0-2.5 kPa), together with the desired stability. In addition, it is also applied to the real-time monitoring of human body movement signals, which showed that the wearable lightweight pressure sensors prepared have good sensitivity and stability.

E1.3

A self-powered intracardiac pacemaker

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Implantable bioelectronic devices play an increasingly important role in disease prevention, monitoring, and treatment. However, it should be noted that the application of implantable bioelectronic devices, including leadless pacemakers, faces various challenges related to power supply in long-term operation due to battery capacity limitations. Besides, leadless pacemakers are costly and difficult to remove after implantation. Here, we report a battery-free, transcatheter, self-powered intracardiac pacemaker (SICP) based on the coupled effect of triboelectrification and electrostatic induction for the treatment of arrhythmia in large animal models. The SICP integrates the energy harvesting unit and power management unit & pacemaker module. We show that the capsule-shaped device (1.75 g, 1.52 cc) can be integrated with a delivery catheter for implanting in the right ventricle of a swine through the intravenous route, which effectively converts cardiac motion energy to electricity and maintains endocardial pacing function during the three-week follow-up period. The material and structural design creates a lightweight, miniature device that maintains stable energy harvesting performance and excellent biocompatibility in vivo. We measure in vivo open circuit voltage and short circuit current of the SICP of about 6.0 V and 0.2 µA, respectively. Meanwhile, the energy harvesting unit is mainly constructed of polymer materials, which provides feasibility for SICP to be compatible with MRI examinations during clinical applications. This approach exhibits up-to-date progress in self-powered medical devices and it may overcome the inherent energy shortcomings of implantable pacemakers and other bioelectronic devices for therapy and sensing.



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E2.1

Self-assemblies of Piezoelectric Metabolites and Their Energy Harvesting Applications

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Piezoelectric metabolite materials have received increasing attention in recent years owing to their inherent biological nature and efficient energy conversion capability, and piezoelectric metabolite self-assemblies are considered as promising smart materials for energy, sensor, robotics, healthcare, and many other areas. Rational material design is important to enhance their piezoelectric and biological activity. Herein, recent advancements to piezoelectric biomaterials, such as amino acids and peptide-based micro/nanostructures, are provided. Synthetic methods, morphological features, and piezoelectric performance of piezoelectric biomaterials on their piezoelectric activity are discussed. The applications of piezoelectric biomaterials in the field of nanogenerators are provided at the end.

E3.1

Revolutionizing Multifunctional Subaquatic Apparatus via Advanced Structural Engineering of Nanocarbon Materials

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A paradigm shift is underway in underwater technology, driven by advanced nanocarbon structural engineering. The age-old challenge of effective underwater adhesion is conquered with a novel approach – a one-way valve design that deftly channels residual liquid away from the adhesion interface, ensuring robust locking and substrate sealing. Crafted from low-dimensional materials like CNT, Graphene, and MXene, this adhesive material features a high-aspect-ratio vertical channel for swift water transport and multiple mesopores that enhance liquid storage efficiency. A remarkable adhesive strength of 216.5 ± 5.5 kPa is achieved, surpassing the 100 kPa benchmark for underwater adhesives. Cycling endurance soars to an unprecedented 100,000 cycles, while a rapid 1.5-second adhesion cycle time sets a new standard. Mechanistic insights unveil the synergy between submicron vertical channels and surface cup area fractions,

amplifying adhesion prowess. Shifting focus to pressure sensors, a groundbreaking self-adhesive sensor emerges, combining aligned and nonaligned carbon nanotube components. It detects pressures as low as 18 mPa with remarkable linearity, while the nonaligned component ensures effective underwater adhesion and secure fixation (Fig. 1). This sensor extends the detectable pressure range by four orders of magnitude, akin to air applications. Fusing artificial neural networks with the sensor achieves flawless underwater target recognition. This transformative narrative marks the dawn of a new era in multifunctional subaquatic technology, driven by ingenious nanocarbon structural engineering [1,2,3].



Fig. 1. Non-contact underwater target detection

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E3.2

Highly Stretchable Self-Powered Piezofibers for Biomedical Applications

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Recent developments in miniaturized electronic devices with higher computational capabilities and ultralow-power communication technologies involve a tendency toward powering these devices with high energy efficiency, long cycle life, fast and cheap manufacturing, and low-weight power sources. Mechanical energy harvesters are needed for diverse applications such as self-powered sensors, human health monitoring systems, and cheaply harvesting energy from human movements. The integration of piezoelectrics and novel fabrication strategies has established the emergence of the wearable technology field, which can meet these needs. In particular, fiber-based electronic devices can be integrated into garments with desirable attributes such as flexibility, stretchability, permeability, and lightweight. Piezoelectric fibers based on polyvinylidene fluoride (PVDF) are an ideal interface platform option between the environment, electronic devices, and the human body, highlighted in the wearable technology field.

Here, we considered methods of fiber formation and developed novel structures (weave, knit, braid, coil) with embedded electrodes. The flexibility and small diameter of the final fiber make it possible to use them in biomedical applications, including sensors and smart scaffolds. The triaxial braided PVDF structure generated a maximum output voltage of 380 mV and a power density of 29.62 μ Wcm⁻³, which is approximately 1559% higher than previously reported for piezoelectric structures.¹ The high-performance hybrid piezofiber of PVDF/barium titanium oxide (BT) nanoparticles was knitted to generate a maximum output voltage of 4 V and a power density of 87 μ Wcm⁻³ under hydraulic and/or pneumatic pressure.² The coiled nanocomposite fibers of PVDF/BT/ reduced graphene oxide (rGO) nanosheets can stretch up to ~100% strain and cause a peak voltage output of ~1.3 V with a peak power density of 3 W kg⁻¹, which is 2.5 times higher compared to previous research. The coil structure shows an energy conversion efficiency of 22.5%.³

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E3.3

Electronic-integrated Textiles Towards Wearable Applications

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The integration of functional electronics into wearable forms, that is wearable electronics, has exhibited vast application possibilities in healthcare monitoring, therapy, and human-machine interactions. With the increasing awareness and growing demand for wearable electronics, more and more attention has been attached to the exploitation of new materials and device structures that only exhibit promising electronics functionalities but also have satisfactory conformability and comfort. While flexible electronics based on thin-film technologies have gained significant progress in terms of device functionalities, performance reliability, and integration ability, only a few research focuses on the realization of bio-compatible, permeable, and comfortable electronics that were of necessary importance for practical wearable or on-skin electronic applications. To address these challenges, electronic functions integrated into textile materials, including fiber, yarns, fabrics, and even clothes, would be one of the promising approaches, which could effectively impart the electronics with intrinsic softness, excellent permeability, and more design form factors. This talk will introduce our research efforts on developing flexible electronic devices based on textile materials and structures. We will discuss the fabrication of fibrous conductive materials including conductive fibers, yarns, and fabrics, as well as their application as building blocks in flexible electronics. In particular, we show the compatible applications of textile technologies in the development of flexible sensing textiles for wearable applications.

E4.1

Biofabricated Advanced Materials for Sustainable Solutions

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Bacterial cellulose (BC) has been explored for use in a wide range of applications including tissue engineering, drug delivery and textile. BC can be produced from various waste streams, but often requires further modification to achieve desirable properties. There is a need to develop sustainable approaches to modify BC to add functionality. Biofabricated advanced materials have emerged as a promising avenue for sustainable solutions in various industrial applications. This study focuses on the in situ bioprocessing modification of bacterial cellulose, a biopolymer renowned for its exceptional mechanical properties and biodegradability, through the utilization of different carbon resources and hydrophobic proteins. The in situ bioprocessing approach allowed for the direct integration of these carbon resources during the microbial synthesis of BC by Komagataeibacter xylinus. This entails not performing any chemical reactions or mechanical processes to change the properties of structure of the BC after the BC has been extracted from the bioreactor. The results showed that in situ modification of BC showed an increased hydrophobicity. The level of hydrophobicity could be controlled and the highest water contact angle recorded was 120°. The results suggest that the strategic modification of bacterial cellulose via in situ bioprocessing with varied carbon resources and hydrophobic proteins can produce advanced materials with tailored properties. This approach not only offers a sustainable method for material production but also expands the potential applications of bacterial cellulose in various industrial sectors.

E4.2

Stretch to Cool: Thermodynamics of Biaxially Strained Natural Rubber for Elastocaloric Heating and Cooling

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According to a 2021 report by the International Energy Agency, heating, and cooling account for roughly 40% of the total energy consumed in Europe [1]. Heat pumps are efficient but rely on refrigerants with high global warming potential [1, 2]. In contrast, solid-state caloric technologies, especially elastocalorics, show great promise in replacing traditional vapor-compression systems [3]. However, current designs for metallic alloy-based elastocaloric devices require high stress (~hundreds of MPa) for an acceptable thermal response, posing an engineering barrier to widespread use [3]. Polymer elastocalorics, on the other hand, are responsive to low-applied strains and have a long service life [4]. However, research on smart polymers for elastocalorics is in its infancy due to a lack of thermo-mechanical characterization and an understanding of the thermodynamics involved in effectively straining a thin polymeric sheet to extract maximum thermal energy [3, 4]. Herein, we experimentally investigated the elastocaloric response of millimetre-thin rubber sheets by inflating and deflating them, thus applying a biaxial strain, as shown in Figure 1(a-d). Additionally, we developed a theoretical model using Gaussian statistical mechanics to explore the thermodynamic mechanisms of entropy change associated with polymer stretching and strain-induced crystallization. Our experimental setup achieved a significant temperature difference of 28°C, with maximum and minimum temperatures of 36°C and 8°C, respectively, using simple natural rubber sheets (Figure 1e). We also discuss how film thickness and fluid-structure interactions affect the timescales of inflation and deflation and highlight the importance of ensuring adiabatic conditions in practical applications. Our theoretical model provides novel insights into the thermo-mechanics of polymer stretching and chain rearrangement, which align well with the experimental results (Figure 1f). Our findings and theoretical framework could pave the way for designing efficient, emission-free elastocaloric heat pumps.



Figure 1: (a-d) Time sequence depicting the spatial variation in the temperature of an inflating and deflating rubber film (thickness 1 ± 0.01 mm); (e) Variation in the temperature of a rubber film as a function of instantaneous strain throughout the inflation-deflation process, illustrating a thermomechanical energy conversion cycle; (f) Comparison between the experimental results and the theoretical predictions of the maximum temperature change as a function of peak strain.

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E5.1

Mechanics of Triboelectric Nanogenerators

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Triboelectric nanogenerators (TENGs) are a promising energy harvesting technology receiving significant global attention at present. This talk will explore the mechanics of TENGs in normal contact separation mode and demonstrate just how mechanics can have an important effect on electrical output. In particular, we focus here on the effect of the following parameters: contact force, 'real' contact area and surface roughness.

Results published in the literature have indicated that TENG electrical output appears to be very sensitive to aspects like contact force and surface roughness. We show that this dependency really results from how the so called 'real' contact area of rough surfaces responds to changes in contact force and roughness [1, 2, 3]. In this talk, we will also explore approaches for *in-situ* measurement of the real contact area. Our TENG tests concurrently measure both TENG electrical output and real contact area over a wide range of contact forces and surface roughness values. Fig. 1 illustrates an optical technique for measuring the real contact area and shows area maps for different surface roughnesses (same force here). The electrical results show that power drops as the contact area drops in line with the surfaces getting rougher. The important implication is that surface topography and contact force must be carefully considered in the design of TENGs and their output can clearly be optimised by optimal selection of surface topography, mechanical properties of the contacting materials and contact force (or pressure).



Fig. 1. In-situ measurement of contact area in triboelectric nanogenerators.

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F1.1

TRANSFORMING AUXETIC METAMATERIALS INTO SUPERHYDROPHOBIC SURFACES

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Auxetic metamaterials defy conventional expectations by expanding laterally when subjected to strain.^{1,2} This unexpected characteristic arises from the arrangement of their lattice rather than the properties of individual solid elements, with the expansion occurring by increasing the space between solid elements. This behaviour offers a pathway for engineering superhydrophobic materials³ with distinct wetting properties which, surprisingly, has not been explored until now. Here, I present theoretical and experimental models predicting and confirming the correlation between different states of strain and superhydrophobicity as a hydrophobic lattice structure is transformed from a negative Poisson's ratio auxetic mechanical metamaterial into a conventional positive Poisson's ratio material (Fig. 1).⁴ I also show how transitions from a superhydrophobic state to a penetrating state can occur as either a superhydrophobic auxetic material is strained or the surface tension of the liquid is reduced.⁵ These results offer a new approach to designing superhydrophobic materials for self-cleaning surfaces, droplet transportation, droplet encapsulation, and oil-water separation.

Acknowledgement. This work has contributions from many co-workers and was funded by the UK Engineering & Physical Sciences Research Council (EP/T025158/1 and EP/T025190/1).



Figure 1. Comparison of theoretical prediction and measured changes in contact angle for different states from auxetic to conventional for a hydrophobic bowtie lattice.

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F1.2

Crafting Next-Generation Functional Membranes through Unconventional Chemical Syntheses

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In this presentation, I will outline two innovative synthetic methodologies for functional membranes developed by our team. The first methodology employs photochemical techniques to create superwettable hybrid membranes, which are particularly effective for oil/water separation. This process utilizes ZnO nanoparticles as a multifunctional agent to initiate a spatially controlled photopolymerization. Additionally, these nanoparticles enhance surface roughness, contributing to the membrane's superwettability. The resulting porous membranes can be engineered to be either superhydrophobic or superhydrophilic, making them versatile for various applications including water treatment, oil spill remediation, and oil purification. This method demonstrates several important advantages, such as versatility for different applications, scalability, exceptional oil/water separation efficiency, and the potential for integration with additional water purification functionalities.

The second part of my presentation introduces a novel technique for synthesizing cross-linked membranes at the interface of a strong acid. This unique 'on-acid' membrane synthesis capitalizes on the assembly of negatively charged surfactants at the acid/air interface, which in turn electrostatically draws protonated monomers to this interface. This strategy differs from traditional aqueous phase interfacial polymerization and greatly expands the scope of possible chemistries for new functional membranes. The method paves the way for next-generation membranes with unparalleled functionality and enhanced durability.

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F1.3

Precision interfacial engineering for fouling and pollution control

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Nanoengineering of non-wetting surfaces offers a promise to widen their application, which nearly always have multiple competing functional requirements. However, the challenges around sustainability, energy-efficiency, robustness, etc. continue to remain major bottlenecks to progress. In this presentation, we will discuss the need for precision and scalability in surface manufacture, with an emphasis on surfaces for controlling (bio)fouling which impairs a large number of energy and propulsion systems. The biofouling issue is also linked with antimicrobial resistance (AMR), a major healthcare challenge. The role of substrate mechanical properties will also be discussed by drawing from recent advances in flexible non-wetting surface designs which enhance the liquid impact resistance property of such surfaces. An extension of this strategy will then be discussed, specifically focussing on pollution control applications. Next, I will share some perspective on how interfacial nanoengineering may need to evolve to meet future human healthcare and net zero aspirations in infrastructure resilience, built environment and transport applications. To this end, we will discuss recent progress around replacing poly- and perfluoroalkyl substances (PFAS) – ingredients in wide-spread use in non-wetting surfaces synthesis but with major ecological and human health harm potential – using metal and covalent organic frameworks, and introducing sustainably sourced materials.

F2.1

Wetting of Droplets on Lubricated Surfaces

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An important goal in research into wetting phenomena is to design surfaces that repel any kind of liquid. Recently, inspired by pitcher plants, there has been a surge of interests in lubricated surfaces whereby rough, porous, or textured materials are infused with lubricants [1,2]. This gives rise to highly slippery surfaces that are promising for a wide range of applications, including for self-cleaning, drag reduction, anti-icing, and anti-fouling. Here we present our recent works using the lattice Boltzmann method to model droplet wetting on and moving across such lubricated surfaces. Unique to these surfaces is that the droplet is surrounded by a lubricant wetting ridge. The presence of such lubricant ridge leads to different static and dynamic wetting behaviors when compared to non-infused dry solids [3-5], including a new description for the contact angle and friction law, as well as a novel bidirectional droplet self-propulsion. We further explore the case where the solid textures are infused by two immiscible lubricants with different levels of wettability that separate into periodic liquid domains. The balance of interfacial tensions between the droplet, the surrounding gas, and the two lubricants leads to multiple possible wetting states, which are distinguished by whether the lubricants cloak one another and/or the droplet.

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F3.1

Nature-inspired Hierarchical Multifunctional Soft Materials

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Soft polymer materials have emerged as versatile materials for flexible electronics and soft robotics, owning to their great stretchability and biocompatibility. However, most soft materials still encounter difficulties in meeting the demanding requirements of real-life applications due to the long-standing challenge of reproducing the excellent mechanical properties and multifunctionalities observed in natural soft tissues. Mammalian skin, for example, exhibits excellent tearing resistance and flexibility due to an intricate hierarchical structure of collagen fibers and fibrils. The hierarchical organization of tendons endows them with high strength and flexibility, allowing them to endure mechanical stress and execute contractions and relaxations. Inspired by the remarkable properties of bio-soft tissues, we have developed various multiscale manufacturing technologies to produce hierarchical soft materials with high mechanical properties and multifunctional capabilities. This involves a freeze-casting solution substitution strategy, a facile combining strategy of self-assembly and stretch training, and a self-assembly-induced bridge crosslinking strategy. The strength of our materials has increased from 6.5 MPa, 20.78 MPa, and 54.8 MPa, while the toughness has also increased from 58.9 MJ/m³, 153.97 MJ/m³, to 260 MJ/m³, owning to multiple strengthening and toughening mechanisms at different scales. We have demonstrated the potential applications of our materials for monitoring sport behaviours in soccer training, non-contact speaking detection, and controlling artificial arms for grabbing objects, etc.

F3.2

Transforming 2D to 3D: Mechanics Principles Enable Shape-Morphing

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The ability of an object to change its shape is as important to an emerging class of engineering applications as it is to biological organisms: just as animals and plants morph in response to external stimuli, soft robots must be able to change shape to adapt to different environments and to complete different tasks. Artificial structures with the ability to change their shapes are referred to as shape-morphing structures. A number of shape-morphing mechanisms have been proposed in recent years. However, due to the restriction of geometric incompatibility, it remains challenging to achieve a three-dimensional (3D) target structure with the desired geometry from a two-dimensional (2D) flat sheet, especially lacking the inverse design framework [1]. In addition, achieving a particular 3D shape usually requires multiple responsive materials and/or the application of external stimuli. In this talk, I will showcase several examples that demonstrate how architected materials can be utilized to create shape-morphing structures with complex geometries through simple mechanics principles.

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F3.3

Ultrathin gas-permeable electronic skins for health monitoring

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One limitation of commercialized wearables, such as smartwatches and bands, is that they cannot form conformable contact with human skin due to their rigid form factor, thereby limiting their monitoring capabilities. Soft bioelectronics, on the other hand, is touted as an ideal platform for personalized health care owing to unique characteristics, such as thinness, lightweight, good biocompatibility, excellent mechanical robustness, and great skin conformability. Permeable skin-mountable electronics capable of long-term applications have emerged as promising tools for early disease prevention, screening, diagnosis, and treatment. Dr. Wang's research interests mainly focus on developing wearable electronics for biomedical health monitoring, including stretchable conductors, sensors, and soft energy devices. In today's talk, she will introduce high-performance skin bioelectronics developed by ultrasoft nanomesh systems, which can realize the accurate measurement of minus skin deformations and finger touch without disturbing natural skin motions and sensations, as well as long-term applications for health monitoring.



Figure 1. Evolution of nanomesh-enabled ultrathin gas-permeable electronic skins.

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F4.1

Bioprinting functional living materials based on granular hydrogels

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F4.2

Intelligent skin electronics for human machine interface and healthcare monitoring

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Soft bio-integrated electronics have attracted great attentions due to the advantages of soft, lightweight, ultrathin architecture, and stretchable/bendable, thus has the potential to apply in various areas, especially in the field of biomedical engineering. By engineering the classes of materials processing and devices integration, the mechanical properties of the flexible electronics can well match the soft biological tissues to enable measuring bio signals and monitoring human body health.

In this report, we will present materials, device structures, power delivery strategies and communication schemes as the basis for novel soft bio-integrated electronics. For instance, we will discuss a wireless, battery-free platform of electronic systems and haptic interfaces capable of softly laminating onto the skin to communicate information via spatio-temporally programmable patterns of localized mechanical vibrations[1-2]. The resulting technology, which we refer as epidermal VR, creates many opportunities where the skin provides an electronically programmable communication and sensory input channel to the body, as demonstrated through example applications in social media/personal engagement, prosthetic control/feedback and gaming/entertainment. Other demonstrations will include skin-interfaces human machine interface for robotic VR, skin like patches as sensors for healthcare monitoring and energy harvesting, etc.[3-6]

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Invited Oral ABSTRACTS

A1.4

"Smart" Pellets: A New Perspective on Heterogeneous Catalysis?

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Heterogeneous catalysts play a crucial role in various industrial processes, significantly impacting both the economy and society. However, their effectiveness is often limited by diffusion constraints within the random pore network of catalyst pellets. While engineering solutions can partially mitigate these issues, our research aims to provide a comprehensive solution by introducing an anisotropic pore structure, termed "Smart" pellets (Figure 1). This innovative approach aims to overcome the long-standing limitations of conventional catalysts, significantly enhancing diffusional transport, catalyst utilization, and reaction efficiency. The implications of this breakthrough extend to material innovations in metal, ceramic, and organic-inorganic composites, advancements in catalyst and reactor technology, and diverse applications across industries.



Figure 1. Innovative Smart pellets for intensified reaction or adsorption processes

In this work, we will showcase the use of alumina pellets with such an asymmetric pore structure, loaded with cobalt, for advanced oxidation processes (AOPs) to address emerging organic pollutants in water. Our findings align with the enhanced diffusional mass transfer, thereby improving the catalytic performance. We will also outline our plans and ongoing research centered on Smart pellets in areas such as Fischer-Tropsch (FT) synthesis and Carbon Capture and Utilization (CCU), among others. Additionally, we will discuss our pilot-scale system for producing ceramic hollow fibre membranes, the First of a Kind (FOAK) in the UK and EU. We anticipate the development of new academic and industrial collaborations in both the catalysis and membrane areas and therefore contribute to renewable energy, the circular economy, and a sustainable future.

A2.2

Electrochemical Performance of Novel Poly (O-toluidine) Based Transition Metal Oxide Nano-composites as Efficient Storage Materials for Super-capacitors

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In the present era, one of the world-wide issues that have received immense attention of researchers, academia is the energy crises. Electrochemical energy storage materials are considered to be one of the solutions to resolve this issue. These are used as electrode materials for electrochemical super-capacitors (ECs). ECs are devices with high charge storage capacity and greater % capacitance. In this work, we fabricated POT based WO₂, CeO₂ and Fe₂O₃ nano-composite materials through one pot blending and emulsion polymerization. UV-Vis study shows different electronic excitation (π - π * and n- π *). FT-IR spectra revealed the inclusion of reinforcement particles inside the polymer matrix through the engagement of the polymers functionalities via metal oxide components. SEM studies explained different morphologies like spherical, rod, porous and pellets shaped of the fabricated composites. The particle size was found in the range from 50-90nm. Cyclic voltammetry (CV), Galvan static charge discharge (GCD) and electrochemical impedance spectroscopy were uses to determine the electrochemical characteristics of the materials. After intensive examination, it was found that the produced materials are highly efficient with about 510.34 F/g charge storage capacity and about 75-80% capacitance retention. The materials displayed high energy density up to 1800.10 Wh/kg. The materials are supposed to be efficient high enough for the fabrication of electrodes for ECs on commercial basis.

A2.3

Entropy-driven Direct Air Electrofixation

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According to the rule of chemical thermodynamics, the catalytic activation of small molecules (like N₂ in air and CO₂ in flue gas) generally exhibits a negative activity dependence on O₂ owning to the competitive oxygen reduction reaction (ORR). Nevertheless, some catalysts can show positive activity dependence for N₂ electrofixation, an important route to produce ammonia under ambient condition. Here we report that the positive activity dependence on O₂ of (Ni_{0.20}Co_{0.20}Fe_{0.20}Mn_{0.19}Mo_{0.21})₃S₄ catalyst arises from high-entropy mechanism. Thorough experimental and theoretical studies, we demonstrate that under the reaction condition in the mixed N₂/O₂, the adsorption of O₂ on high-entropy catalyst contributes to activating N₂ molecules characteristic of elongated N≡N bond lengths. As comparison to the low- and media-entropy counterparts, high entropy can play the second role of attenuating competitive ORR by displaying a negative exponential entropy-ORR activity relationship. Accordingly, benefiting from the O₂, the system for direct air electrofixation has demonstrated an ammonia yield rate of 47.70 µg h⁻¹ cm⁻², which is even 1.5 times of pure N₂ feedstock (31.92 µg h⁻¹ cm⁻²), overtaking all previous reports for this reaction. We expect the present finding providing an additional dimension to high entropy that leverages systems beyond the constraint of traditional rules.

A3.4

Harnessing Acoustic Cavitation for Initiating Frontal Polymerization Through

Activation of Grubbs' Second-Generation Catalyst

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Energy-efficient manufacturing processes are crucial for sustainable and cost-effective production of high-performance polymers and composites.¹ Frontal polymerization (FP) has emerged as a promising method for the rapid synthesis of polymers. FP is a unique method that relies solely on external energy to overcome the energy barrier required for initiating exothermic polymerization, leading to the formation of a self-sustained reaction zone known as the "polymerization front".^{2–4} However, the pursuit of improved mechanical properties, scalability and safety concerns necessitates alternative efficient initiation strategies. Here, we introduce a novel method to initiate FP by harnessing ultrasound mechanical waves instead of thermal initiation. According to the hotspot theory, the fast collapse of microscopic bubbles during cavitation can result in high pressures and intense local heating with short lifetimes. These powerful and highly concentrated hotspots can be used to initiate energetic chemical processes such as affecting the ROMP catalyst.⁵ In the model NMR experiments, new ruthenium species could be observed after ultrasound irradiation for 30 seconds meaning that ultrasound-induced FROMP (U-FROMP) was initiated via the metathesis of Grubbs catalyst (G2) via necessary ultrasonication. It was further confirmed that instead of relying solely on heat generation, ultrasound was crucial in activating the G2 catalysts. It is observed that the initial ultrasound amplitude influences mechanical properties with the regulation of frontal temperature, polymer micro-, and nanostructure. At optimum ultrasound amplitude, with a 55 °C decrease in frontal temperature compared to the thermal FROMP, the tensile yield strength and ductility of the polymers are improved, leading to enhanced plastic deformation and a remarkable 336% improvement in toughness compared to the thermal FP. These findings highlight the significance of manipulating ultrasound factors to exert control over the network structure of polymer.

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A4.3

An Overview of Renaissance of Artificial Intelligence in Material Science

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Artificial intelligence (AI) has become a disruptive force in many industries over the past few decades, and the subject of material science and engineering is no exception. The tremendous effects of AI on material innovation, design, prediction, and synthesis are examined in this review study. The time-consuming and ineffective nature of conventional trial-and-error procedures in materials research is well known. However, AI has ushered in a new era of increased productivity because to an abundance of training data, improved computer power, and sophisticated deep learning algorithms. The use of AI in material design is distinguished by its capacity to identify complex correlations and patterns within large datasets, allowing the prediction of material characteristics and behaviours. Additionally, AI-driven models are excellent at predicting the performance of materials, which is crucial in sectors where exact material specifications are required. AI has an impact on material synthesis in addition to design and forecasting. It manages and optimizes the synthesis procedure to effectively generate materials with the desired qualities. This paper focuses on the specific methodologies and advantages AI provides over traditional approaches in applications related to material science. The speed with which AI can scan enormous data sets, find hidden patterns, and adjust to new information dramatically cuts down on research costs and timetables. The paper explores how AI will develop in material science in the future, including how algorithms will be improved, integrating exceedingly intricate simulations. A future of quick innovation and discovery is promised because of the synergy between AI and material science. Lastly, this page explores potential challenges and pitfalls in using AI in Material Science, including ethical and technical considerations amongst others.

B4.3

TITLE TBD

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B2.2

Electrosynthesized Poly(3-fluorothiophene): Tough Intermolecular Network for High-performance Electrochromic Supercapacitors

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Electrochromic supercapacitors (EC-SCs) have already attracted considerable attention for their applications in flexible electronic devices[1,2]. However, despite recent encouraging progress, rational design and development of EC-SC materials with high-performance remain challenges in this field[3,4]. Here, we proposed a fluorination strategy to develop EC-SC materials with tough intermolecular network obtained by one-step electrosynthesis of 3- fluorothiophene for flexible electrochromic supercapacitors. The poly(3-fluorothiophene) (PFT) films simultaneously achieved high electrochromic performance (optical contrast 42% at 560 nm), and good capacitance property (290 F g⁻¹, 1 A g⁻¹), as well as outstanding cyclic stability (<2% reduction after 20,000 cycles). Enabled by the PFT, flexible electrochromic supercapacitor changes during charging/discharging, which can be used to visually monitor the energy storage state in real time and still maintain good performance under bending state. This fluorination strategy will provide a new design idea for high-performance EC-SC materials to prepare reliable FESDs.



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B2.3

Intercalation-type electrode materials for calcium rechargeable batteries

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The growing demand for electric vehicles and stationary energy storage systems calls for developing next generation batteries that combine high energy, high power and low cost. Among many post lithium-ion batteries, calcium rechargeable batteries utilizing divalent Ca^{2+} ion charge carriers are expected to offer clear benefits in affordability and potentially high energy density, due to the abundance of calcium in the Earth's crust (46600 ppm *versus* 20 ppm for lithium) and the low redox potential of Ca/Ca^{2+} (-2.9 V *vs.* standard hydrogen electrode). However, the lack of suitable electrodes is the Achille's heal of the calcium rechargeable battery technology. The relatively large ionic radius and divalent nature of Ca ions make the insertion kinetics generally sluggish in intercalation hosts. Moreover, a large Ca^{2+} intercalation is supposed to cause extended volume changes, triggering a premature degradation of electrode structures. In this talk, I would like to present our recent work in exploring intercalation-type electrode materials for high-performance calcium batteries. The new calcium ion storage mechanisms and landmarking performance will be highlighted. Finally, I would like to discuss on the outlook of non-aqueous calcium rechargeable batteries.

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B3.4

Conductive polymer decorated zinc azelate Bio-MOFs as high performance supercapacitors

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The rapid technological advancements drive a growing demand for energy, urging researchers to develop high-performance clean energy devices using renewable and sustainable materials. Supercapacitors, also known as electrochemical capacitors, are crucial energy storage devices delivering power from diverse sustainable sources. Their remarkable features including high power density and cyclic stability, make them highly desirable. Metal organic frameworks (MOFs) represent successful materials for investigating high energy density systems due to their large surface area, three-dimensional porous architecture, structural diversity, and mechanical and chemical stability. However, the low electrical conductivity of MOFs limits their application in energy storage devices. Combining MOFs with conductive polymers (CPs), is a strategic approach to enhance specific capacitance and overall performance.

In this study, we synthesized and characterized conductive biodegradable polymer functionalized Zincbased Bio-MOFs as electrode materials for high performance supercapacitor. Bioactive azelaic acid served as organic linkers to Zn metal ion, introducing antibacterial activity to the MOFs. Polypyrrole (Ppy) and polyaniline (PANI) were chosen as bio-degradable conductive polymers for decorating Bio-MOFs. The chemical features of the composite materials were analysed using XRD, FTIR, TGA, and XPS techniques. SEM and TEM microscopic analysis revealed platelet structures of MOFs decorated with nanospheres of CPs. Electrochemical studies in three electrode system using 0.5M Na₂SO₄ as electrolyte solution demonstrated that CP decorated Bio-MOF composite exhibited 3 folds higher electrochemical capacitance and improved cyclic stability compared to the parent Bio-MOF as supercapacitor electrode materials. The observed high supercapacitance is attributed to the synergistic effect of zinc azelate Bio-MOF and CP nanoparticles in the composite matrix.

B1.4

High-Throughput Screening Design of Novel Molten Salts of Energy Storage Based

on Machine Learning Property Prediction Models

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Molten salt energy storage, as an environmentally friendly energy storage technology, plays a significant role in today's energy transition and sustainable development. Molten salts are the most widely used storage and heat transfer medium in the field of solar thermal power generation. In recent years, driven by the global demand for stable new energy development, the design of novel molten salts with a wider temperature range has garnered extensive attention¹. In materials design, data-driven research paradigms have shown promising applications as replacements for the traditional experimental "trial and error" approach². However, the application of this method in molten salt design has not been deeply studied or widely promoted³.

This work established an energy storage molten salt database based on experimental data and publicly published literature, followed by data mining and machine learning model construction. Through high-throughput screening, this approach ultimately enables the efficient design of target molten salts. Selection and optimization of 6 commonly used machine learning models in the field of material prediction were conducted. The final models exhibit stable and reliable performance in predicting the melting points and decomposition temperatures of multicomponent molten salts. The resulting models demonstrate stable and reliable performance in predicting the melting points and decomposition temperatures of multicomponent molten salts. The resulting models demonstrate stable and reliable performance in predicting the melting points and decomposition temperatures of multicomponent molten salts. For the test set, the coefficient of determination (R²) of the melting point prediction model exceeds 0.85. In a self-constructed design space of 748,157 virtual molten salt formulations, eight novel molten salts were screened out, with the maximum usable temperature range extending 150°C beyond that of the currently commercial Solar Salt. This work demonstrates the broad prospects of machine learning-based high-throughput screening methods in the field of molten salt design for novel thermal energy storage systems.

C1.3

Techno-economic Analysis of Direct CO₂ Capture from Air Integrated with Utilisation

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The Paris Agreement has set an aim that global warming should be limited to 1.5 °C by 2100, thus carbon neutrality should be reached by 2050 [1]. To achieve this goal, direct air CO₂ capture (DAC) and storage (DACCS) have the potential to achieve net-zero emissions due to their availability of low CO₂ levels. Despite the fact that DAC/DACCS are relatively new and in early commercial stages, in a long-term perspective, it is still essential to develop further application as they can help control and mitigate climate change [2]. Therefore, considering that Carbon Capture and Utilisation (CCU) can contribute to a green carbon circular economy by replacing fossil carbon value chains, Direct Air Carbon Capture and Utilisation (DACCU) is emerging as a renewable route to allow full circularity of CO₂ and water. However, there are still many technical challenges such as energy penalties, stability and large cost. Recently, reported Integrated Carbon Capture and Utilisation (ICCU) was designed to simplify the CCU process as much as possible [3]. This ICCU technology can promote CO₂ conversion with fewer intermediate steps, leading to a reduction in overall cost and energy consumption [4]. In this research, ICCU is applied to DAC, to form a novel direct air carbon capture process, DAC- ICCU. According to this innovative concept, this paper will be discussed in detailed techno- economic analysis to determine if DAC-ICCU could reduce the high cost and energy consumption by comparing to conventional DAC, DACCS, and DACCU.



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C2.2

Levelized Cost Analysis of Indirect Evaporative Cooling in Data Centre

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The cooling requirement in data centres have increased tremendously due to the high demand of data processing and storage etc. The energy consumption of cooling requirement in data centre accounts for around 40%. Mechanical vapor compression cooling technology holds a dominant position in the current cooling market, characterized by its energy-intensive nature. However, Indirect evaporative cooling has the potential to gain more market share with the advantage of energy economic and environmental friendliness.

The aim of this research is to analyse economic performance and energy consumption of the traditional mechanical vapor compression cooling system and novel indirect evaporative cooling systems in data centre applications. The study conducts an analysis to discuss costs and potential energy savings. Moreover, it provides suggestions for data centre industry stakeholders to help fulfil the UK net-zero target.

C2.3

Conducting Polymer Hydrogels for High-efficiency Solar Water Evaporation

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Solar water purification offers an environment-friendly, economical, and energy-saving approach to producing clean water, underscoring its immense potential in sustainable wastewater treatment. Hydrogels, owing to their highly tunable physicochemical properties, have emerged as a forefront and innovative material platform in solar water purification. However, existing hydrogel-based solar evaporators grapple with issues like limited light responsiveness, inferior mechanical properties, moderate evaporation performance, and compromised stability, impeding their practical applications. In order to address these challenges, we have proposed new molecular/phase engineering strategies such as PSS chain engineering, hard-soft chain regulation, bi-continuous phase engineering, etc., to design high-performance conducting polymer hydrogels.1-5 With such strategies, we have successfully developed a series of novel PEDOT:PSSbased conducting polymer hydrogels simultaneously achieving broadband light absorption (nearly 100%), robust mechanical properties, fast evaporation rate (~ 4.45 kg m-2 h-1), high energy efficiency ($\sim 98\%$), and prolonged stability (60 days).3-5 To harness these intriguing properties, we further demonstrate the scalable mass production of such hydrogels, and also their efficacy towards potential applications like efficient desalination/purification of varying seawater and sewage samples with low-to-high salinity, strong acids/bases, heavy metal ions, and organic dyes.3-5 Such design strategies of high-performance conducting polymer hydrogels present promising methodologies and materials basis for efficient seawater desalination and sewage purification.

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C3.4

Fe-Mn doping CaO for Synergistic Carbon Capture and Heat Recovery

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Calcium-based sorbents applied for reversible absorption and release of CO_2 are emerging as promising materials for carbon capture, and storage of waste heat from industry at high temperature. During the carbon capture process, CaO absorbs CO_2 during the carbonation step to form CaCO₃, which is then calcined to regenerate CaO and produce a stream of pure CO_2 for long-term storage or conversion into value-added chemicals. However, during the calcination step, the CaO material can sinter, causing rapid degradation in performance over repeated cycles. This paper presents the synthesis of Ca-based sorbents with enhanced resistance to sintering over repeated cycles of carbon capture and release in packed bed reactor, and improved energy density with respect to unmodified CaO.

Doping Mn and Fe ions into the structure of the Ca-based sorbents improved the resistance to sintering, with the materials maintaining a CO₂ capture capacity of 0.7 g-CO₂ $g_{sorbent}^{-1}$ over 30 carbonation-calcination cycles. The energy density was also improved, to 2.51 kJ $g_{sorbent}^{-1}$ as about 2 times over than unmodified CaO. Loading Fe and Mn onto calcined CaO formed a several unique porous structure, like blade-like microstructure, which can limit the sintering effect in the calcination process. The interaction of Fe and Mn can reduce the activation energy in carbonation and calcination reactions and facilitates formation of oxygen vacancies and enhances CO₂ affinity of sorbents and energy storage.



Figure 1. The fixed-bed reactor for carbon capture

C4.2

Investigation of the influence of initial substrate to biomass ratio on kinetic parameters and sequencing batch reactor performance prediction

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Estimating kinetic parameters such as maximum growth rate (μ_{max}), half saturation constant (K_s), endogenous metabolism coefficient (b) and growth yield (Y) in biological wastewater treatment is vital for designing, optimizing, controlling, and monitoring processes, ultimately resulting in enhanced treatment efficiency, environmental sustainability, and cost-effectiveness. The initial substrate to biomass ratio (S_o/X_o) in biological wastewater treatment can significantly impact kinetic parameters and the overall performance of the treatment process. However, limited literature exists on the impact of S_o/X_o on kinetic parameters, and few studies utilize experimentally derived kinetic parameters from batch tests to predict sequencing batch reactor (SBR) performances. This study investigates how S_o/X_o affects both kinetic parameter values and the SBR performance. Two model wastewaters, glucose and ethanol, were treated in SBRs, with substrate and biomass concentrations measured. Four batch tests at varying S_o/X_o were carried out on each wastewater, measuring the oxygen uptake rate (OUR). OUR profiles were used to estimate kinetic parameters using a mathematical model encompassing substrate consumption, biomass growth, and endogenous metabolism. The results showed significant variations in kinetic parameter values attributed to differing OUR behavior across S_o/X_o ratios. The values of μ_{max} , Y and b showed great dependence on the S_o/X_o where higher μ_{max} and lower values of Y and b were estimated as the S_o/X_o increases and vice-versa. The estimated kinetic parameters were used to predict the steady state performance of the SBRs, which were then compared with experimental data. While substrate removal was accurately predicted for all wastewaters, satisfactory predictions of biomass concentration for both wastewaters were only obtained with the parameters estimated in the low S_o/X_o tests. The results showed performance of the SBR was strongly affected by the values of parameters especially b and Y. Uunderstanding the relationship between S_o/X_o and kinetic parameters is essential for optimizing process design, operation, and performance to achieve desired treatment outcomes.

C4.3

Solar to Formic Acid: Machine learning-based case study

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This study explores the conversion of solar energy into liquid fuel as a means of addressing the current crisis of climate change and contributes towards UK net zero emission law. Production of Formic Acid (FA) as a sustainable energy source by harnessing solar energy is essential for reducing the amount of CO_2 in the atmosphere and fits in with the global trend towards renewable energy sources. A two-electron reduction product of CO₂, formic acid has a lot of potential for use as a hydrogen storage material and as a solar liquid fuel. As a result of its application in direct formic acid fuel cells (DFAC), it is positioned as an environmentally responsible substitute for traditional energy sources, greatly lowering greenhouse gas emissions. The primary goal of this research was to optimise solar energy capture through the integration of a sophisticated dual-axis solar tracking mechanism with a photovoltaic (PV) system. By effectively aligning the solar panels with the sun's trajectory, this system maximises energy absorption and subsequently increases the production of formic acid. It is designed to outperform conventional solar tracking methods. PV system's power output and the subsequent formic acid production were monitored to assess the system's efficacy. To evaluate that, Artificial Neural Networks (ANN) and Support Vector Machines (SVM), two predictive modeling approaches were used. The comparative study showed that SVM significantly predicted better results than ANN to produce formic acid as well as the PV system's power. The results of this study demonstrate the extent to which SVM succeeds in maximizing solar energy systems and progress in the development of sustainable solar liquid fuels like formic acid. Furthermore, this research adds valuable insights into the utilization of solar energy for renewable fuel production, towards climate change issues, and offers Formic acid as a sustainable energy alternative.

D1.4

Investigating the Mechanical Properties, Durability, and Environmental Impact of Partial Cement Substitution with Slag Cement and Rice Husk Ash for Sustainable Concrete Production

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Abstract: The production of cement, a key component of concrete, contributes significantly to carbon emissions, exacerbating environmental degradation. This study explores the feasibility of mitigating this impact by incorporating Slag Cement (SC) and Rice Husk Ash (RHA) as partial substitutes for conventional cement. SC and RHA, as industrial by-products, possess pozzolanic properties that not only enhance concrete performance but also reduce its environmental footprint. The research aims to assess the influence of varying SC and RHA replacements on concrete's mechanical properties, durability, and overall sustainability. Experimental investigations encompassed tests on compressive and flexural strengths, water absorption, and chloride penetration. Sustainability assessments during concrete production quantified environmental benefits through measures such as embodied carbon footprint and life cycle analysis. The study reveals promising avenues for the construction sector to adopt SC and RHA in concrete production with environmental consciousness. Integration of SC and RHA not only diminishes the carbon footprint but also enhances concrete properties. Key findings include a noteworthy 20% increase in compressive strength, improved workability up to a 100 mm slump, and a substantial 50% reduction in carbon dioxide emissions per cubic meter of concrete produced. In summary, the results underscore the positive impact of utilizing SC and RHA as partial cement replacements, showcasing improvements in both concrete performance and sustainability.



Figure: Block Diagram of Proposed work
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D2.2

Efficient perovskite solar cells and light-emitting diodes

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Halide perovskite materials own excellent semiconductor properties, which showed great potential in photovoltaic and emission display. In this talk, I will summarize our recent work in perovskite solar cells (PSCs) and light-emitting didoes (PeLEDs). 1) By charge transport layer and perovskite composition engineering, for the bandgap around 1.5 electron volt, we have achieved over than 26 percent efficiency with the FF around 85 percent of organic-inorganic PSCs; 2) According to reducing the halide segregation, a wide bandgap PSCs with 1.30 V has been achieved, by constructing a tandem solar cells, over than 30% PCE was demonstrated; 3). According to several strategies, such as non-radiative recombination suppression, band structure modulation and charge injection balance, we have achieved over than 25 and 20 percent efficiency electroluminescence in red and blue region, respectively.

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D2.3

Crystallization and Interface Modulation for Flexible and Printed Perovskite Solar Cells

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Perovskite solar cells (PSCs) has been considered as one of the promise and competitive candidate for the next generation photovoltaics owing to their unique photovoltaic properties and a remarkable breakthrough in efficiency. In our group, recent efforts have been devoted to crystallization and interface modulation for achieving efficient flexible and printed PSCs. Through interface optimization and crystallization control, efficient flexible PSCs were achieved with power conversion efficiencies (PCEs) of 19.51% (a record value in 2019)^[1], 21.10% (one of record values in 2021)^[2], and over 24 %^[3], respectively. Furthermore, low-dimensional intermediate phase induced by the methylamine chloride (MACI) additive could effectively regulate the crystallization of perovskite, resulting in a PCE of 23.14% and 21.20% for 0.09 cm² and 1.03 cm² PSCs (Figure 1a), respectively, fabricated via two-step sequential doctor-blading process (Figure 1a). An interface material 2-(N-Morpholino)ethanesulfonic acid potassium salt (MESK) is incorporated as the bridging buried interface layer enable 24.67%-efficiency doctor-bladed PSCs in ambient condition, and the mini-modules with an active area of 11.35 cm² exhibit a typical PCE of 19.45% (Figure 1b)^[4]. Meanwhile, roll-to-roll printing process was developed to fabricated efficient flexible PSCs through interface and crystal morphology optimization^[5]. These results indicate that efficient and stable flexible and printed PSCs and modules could be achieved via crystallization and interface modulation.



Figure 1. (a) Schematic illustration and *J-V* curves of doctor-blading PSCs; (b) Photo and *J-V* curves of doctor-blading PSC mini-module.

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D3.4

Adjoint-Based Optimisation of Tubercle Leading Edge Aerofoils to Revolutionise Wind Turbine Blade Performance

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Inspired by the protuberances on humpback whale flippers, tubercle leading edge aerofoils have drawn significant attention for their potential to delay stall and enhance aerodynamic performance. This study optimises a NACA 0021 aerofoil with tubercle configurations using the cutting-edge adjoint solver method in computational fluid dynamics (CFD). The primary objective is to maximise the lift-to-drag ratio at high angles of attack in the post-stall regime, pushing the boundaries of aerodynamic efficiency.

Validated against experimental data, CFD simulations exhibit a remarkable 2% margin of accuracy for liftto-drag ratio at 18 degrees angle of attack. Employing the adjoint solver, the aerofoil geometry is optimised using a gradient-based approach. The optimisation process yielded an impressive 47% increase in lift-todrag ratio after just 7 design iterations, with the most substantial improvements occurring in iterations 3 and 6.

In-depth analysis of the optimised geometry revealed a reduction in tubercle amplitude and a more concentrated flow towards the centre of the tubercles. The separation bubble was minimised, and the velocity magnitude of the vortices within the bubble was notably reduced, contributing to increased lift and decreased drag. Moreover, the pressure coefficient distribution displayed smoother contours and delayed flow detachment from the aerofoil surface.

This innovative study demonstrates the effectiveness of adjoint-based optimisation in enhancing the aerodynamic performance of tubercle leading edge aerofoils, particularly at high angles of attack of the stall region. By pushing the boundaries of aerofoil optimisation, this research paves the way for the development of more efficient wind turbines in future.

D4.3

Polymer of Intrinsic Microporosity Enabled pH-Responsive Adsorptive Membrane: Selectivity and Mechanism

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Molecular separation process is crucial as it involves our daily activities and various industry, such as water purification, energy generation and storage^{1,2}. Amongst diverse separation technologies, membrane-based separation has garnered significant attention due to its efficiency, reduced energy consumption, and simplicity¹. Adsorptive membranes, a novel subset of membrane technologies, ingeniously combine adsorption with membrane separation. These membranes offer a promising solution to challenges associated with traditional pressure-driven membranes, such as energy demands, selectivity/permeance trade-off, and fouling issues. Nevertheless, the practical implementation of adsorptive membranes remains hindered by their restricted processing rates. To propel their development and industrial adoption, enhancing the adsorption capacity of such membranes is paramount.

Polymers of Intrinsic Microporosity (PIMs), pioneered by Budd and McKeown in 2004, are characterized by their distinct microporosity derived from inefficient polymer chain packing. A noteworthy advancement involves the modification of the nitrile group in PIM-1 to the amidoxime group. This alteration not only enhances the hydrophilicity but also broadens the solvent compatibility, positioning the modified PIM-1 as a more suitable candidate for membrane fabrication in liquid separations^{2,3}. We designed and fabricated a pH-responsive amidoxime modified polymer of intrinsic microporosity (AOPIM) membrane for selective separation of charged dyes under varying pH conditions. Utilizing the amidoxime group as the selective affinity site, the AOPIM membrane manifested charge reversals, enabling high adsorption capacity, notably with methylene blue (MB) uptake reaching 444.2 mg g⁻¹. In dye filtration, it achieved substantial separation efficiencies for both anionic (IC: 94.7 L m⁻²h⁻¹bar⁻¹; 80% rejection) and cationic dyes (MB: 94.9 L m⁻²h⁻¹bar⁻¹; 99% rejection). Furthermore, the AOPIM membrane also possess high separation selectivity for cationic dye in dual dye mixture at high pH environment. Results reported here underscores the unique pH-responsive property of the AOPIM membrane, shedding light on the application of adsorptive membranes for pollution control.

E1.4

Multifaceted Improvements in Soil Characteristics and Molecular Dynamics through Inorganic and Bio-Based Nano Additives

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Abstract: Soil is an essential component in the maintenance of terrestrial ecosystems, and plays a pivotal role in agricultural productivity and environmental sustainability. In response to escalating concerns surrounding soil degradation and the imperative for sustainable agriculture, nano additives have emerged as pioneering solutions with transformative potential. This study delves into the intricate dynamics of inorganic and bio-based nano additives, over conventional soil treatments and enhancement strategies. Inorganic nanoparticles, including silica and titanium dioxide, alongside bio-based counterparts like chitosan and cellulose, represent a paradigm shift in soil science. A comprehensive assessment, encompassing pH modulation, moisture retention capacity, aggregate stability, nutrient bioavailability, and microbial dynamics, monitored over a specific timeframe. Characterization techniques such as scanning electron microscopy (SEM) and Fourier-transform infrared spectroscopy (FTIR), showed complex interplay between nano additives and soil constituents, offering unprecedented insights into their synergistic effects. Our findings reveal the enhancement in soil functionality, with nano-clay (1% concentration) with a remarkable 25% increase in aggregate stability, underscoring its pivotal role in fortifying soil structure against erosive forces. Nano-silica (0.5% concentration) emerges as a gamechanger, augmenting water retention capacity by 15%, thereby mitigating drought-induced stress and fostering resilience in agroecosystems. Concurrently, nano-scale biochar (3% concentration) elicited a notable 20% amplification in soil organic matter content, accentuating its potential as a potent carbon sink and enhancer of soil fertility. The universal stimulation of microbial activity across all nano additives, with nano-silica exhibiting a discernible prowess, precipitating a significant 30% surge in microbial biomass carbon. This phenomenon underscores the pivotal role of nano additives in fostering soil biogeochemical cycling and ecosystem functioning, thereby underpinning their instrumental role in sustainable soil management practices. The present research unveils the transformative potential of nano additives in augmenting soil fertility, resilience, and ecosystem health, propelling them to the forefront of contemporary soil science and advocacy for sustainable agricultural practices.



Figure: Fourier-transform infrared spectroscopy (FTIR) spectrum depicting molecular dynamics and compositional changes in soil samples post-nano addition

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E2.2

BIOGENIC METHANE PRODUCTION USING ORANGE (*citrus sinensis*) WASTE CO-DIGESTED WITH ANIMAL FEED STOCKS Sadiya Salihu Umar¹, Usman Mohammed Ibrahim², Sani Ibrahim², Ahmad Abubakar Ishak³

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Anaerobic digestion process of orange waste and animal dung feed stocks was investigated in this study. The study was carried out at mesophilic temperature range of 35-40°C for a retention period of 30 days. Microcosm investigation of biogas from processed orange waste, donkey dung, cow dung and horse dung with molecular amplification of methylcoenzyme-M-reductase (mcrAgene) using universal bacteria archeal 16SrRNA gene for the detection of biogas-producing microorganism (methanogens) were analyzed. Three treatment(s) were established for the study coded orange waste ratio cow-dung (OW:CD), orange waste ratio donkey dung (OW:DD) and orange waste ratio horse dung (OW:HD). Qualitative and quantitative biogas production was estimated. The results of the study revealed that treatments OW:CD and OW:DD had the highest record of biogas produced at 552cm³ and 605cm³ with pH ranges at 4.13-7.9 and 3.99-6.98 respectively. The biogas produced in all the three treatments were flammable when subjected to flammability test. Therefore, the co-digestion of orange waste with animal dungs has the potential of mitigating environmental pollution while producing biogas.

E3.4

BIOGAS PRODUCTION USING ANAEROBIC DIGESTION OF AGRICULTURAL VEGETABLE (CABBAGE AND SPINACH) RESIDUES

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Microbial energy technologies employ microorganisms through the breakdown of organic materials to transform chemical energy in biomass into energy-bearing fuels. Biogas is a product of fermentation from biodegradable materials which serves as profitable means of reducing or even eliminating the menace and nuisance of urban wastes while serving as a reliable source of renewable energy. This study used Agricultural residues of spinach, cabbage and cow dung as substrates through several interdependent, complex sequential and parallel biological reactions in the absence of oxygen. Seven treatments were prepared while temperature, pH, and proximate compositions (moisture, ash content, volatile compounds, fixed carbon, nitrogen and crude fibre) were recorded at 24 hours intervals for 30 days. The results indicate rapid increasing gas production within the first ten days with the exception of a treatment that comprised mixture of cabbage and cow-dung. The highest volume of biogas (1346.552 cm³) was obtained from the treatment of cow dung followed by mixture of the three substrates with 1232.759 cm³ biogas composition. All components of the biogas were confirmed using the GC-MS analyses. Temperature values above 40°C were noticed throughout the experiments while pH values were entirely acidic. All the bacteria isolates obtained belonged to the categorise of Staphylococcus, Bacillus and Proteus species. This shows vegetable waste can be utilized by microorganisms for sufficient biogas production. Utilization of such substrates could be as a result of accessibility by the identified bacteria. Hence, the species played a vital role in biogas production from vegetable wastes.

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E4.3

Emergent Hyper-reflectivity in Cholesteric Liquid Crystals with Facile Stratification-based Strategy

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Cholesteric liquid crystals (CLCs) are chiral photonic materials with selective reflection in terms of wavelength and polarization. Helix engineering is often required in order to produce desired properties for CLC materials to be employed for beam steering, light diffraction, scattering, adaptive or broadband reflection. Here, we demonstrate a novel photopolymerization-enforced stratification (PES)-based strategy to realize helix engineering in a chiral CLC system with initially one handedness of molecular rotation throughout the layer. PES plays a crucial role to drive the chiral dopant bundle consisting of two chiral dopants of opposite handedness to spontaneously phase separate, and create a CLC bilayer structure that reflects left- and right-handed circularly polarized light (CPL). The initially hidden chiral information therefore becomes explicit, and hyper-reflectivity, i.e., reflecting both left- and right-handed CPL, successfully emerges from the designed CLC mixture. The PES mechanism can be applied to structure a wide range of liquid crystal (LC) and polymer materials. Moreover, the engineering strategy enables facile programming of the center wavelength of hyper-reflection, patterning, and incorporating stimuli-responsiveness in the optical device. Hence, the engineered hyper-reflective CLCs offers great promises for future applications, such as digital displays, lasing, optical storage, and smart windows.

F1.3

Programmable and flexible fluorochromic polymer microarrays for information display

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Photo-responsive fluorochromic materials are regarded as an effective means for information storage, their reversible changes of color and fluorescence facilitate the storage process and increase the storage capacity. Here, we propose an optically reconfigurable Förster resonance energy transfer (FRET) process to realize tunable emissions based on photochromic spiropyran and fluorophore. The kinetics of the photo-isomerization of spiropyran, the FRET process of the composite are systematically investigated. Through tuning the ratios of the acceptor spiropyran and donor fluorophore upon external light stimuli, a programmable FRET process is developed to obtain tunable outputs. More importantly, flexible microarrays are fabricated from such fluorochromic mixtures by inkjet printing (230 ppi). The dynamic FRET process can also be constructed and generate tunable fluorescence in the ready-made microstructures. These created flexible patterns based on the functional microarrays can be used as novel optically readable media for information storage by designing the composition and optical performance of every feature within the microarrays. Almost all aspects of information storage such as data recording, anticounterfeiting and colorful display can be integrated into this simplicity and straightforwardness system. The reliable fabrication and programmable optical performances of this large-scale flexible polymer microarray represent a substantial step towards high-density and high-security information storage platforms.



F2.2

Advanced Engineering Materials: Metamaterials

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Metamaterials belongs to the class of advanced engineering materials which are artificially engineered and belongs to a class of smart materials whose design and functionality can only be limited with limited human creativity and imagination. Metamaterials behave in manners that are completely different from the behaviour of conventional naturally accruing materials. For example, the type of metamaterials that interacts with light in such a manner that the light is bent in the opposite direction to what can be observed in natural materials. That is, negative index of refraction. In the same manner, metamaterials can be designed to have negative stiffness, negative mass and negative Poisson's ratio and to interact with sound, heat, or magnetic field in a way that reflect an unprecedented material behaviour. This advanced engineering material gain its property from the artificially designed structure other than the chemical composition that the material is made up of. Additive manufacturing technology, and advance manufacturing technology, can produce any shape no mater the complexity by just adding materials layer after layer is an important manufacturing technology that made the endless design and fabrication of metamaterials a possibility. This novel material has gained a lot of attention in the research community owing to their unprecedented behaviour in service. One of the important areas of application of metamaterials energy harvesting application. Metamaterials can be designed to manipulate input wave direction and amplify strain levels on energy conversion materials. For example, mechanical metamaterials can interact intelligently with mechanical wave energy, converting it into useable electrical energy that harvested more efficiently when compared to naturally occurring or conventional materials. This article explains the brief history of metamaterials, types of metamaterials, properties of metamaterials, the areas of application of metamaterials and in energy harvesting. The use of additive manufacturing technology in manufacturing of metamaterials is highlighted.

F2.3

Shape Morphing of Hydrogels by Harnessing Enzyme Enabled Mechanoresponse

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Hydrogels have been designed to react to many different stimuli which find broad applications in tissue engineering and soft robotics. However, polymer networks bearing mechano-responsiveness, especially those displaying on-demand self-stiffening and self-softening behavior, are rarely reported. Here, we design a mechano-controlled biocatalytic system at the molecular level that is incorporated into hydrogels to regulate their mechanical properties at the material scale. The biocatalytic system consists of the protease thrombin and its inhibitor, hirudin, which are genetically engineered and covalently coupled to the hydrogel networks. The catalytic activity of thrombin is reversibly switched on by stretching of the hydrogels, which disrupts the noncovalent inhibitory interaction between both entities. Under cyclic tensile-loading, hydrogels exhibit self-stiffening or self-softening properties when substrates are present that can self-assemble to form new networks after being activated by thrombin or when cleavable peptide crosslinkers are constitutional components of the original network, respectively. Additionally, we demonstrate the programming of bilayer hydrogels to exhibit tailored shape-morphing behavior under mechanical stimulation. Our developed system provides proof of concept for mechanically controlled reversible biocatalytic processes, showcasing their potential for regulating hydrogels and proposing a biomacromolecular strategy for mechano-regulated soft functional materials.

F3.4

Development of Robust and Durable Superhydrophobic Surfaces through Lasertextured Micro/Nano Armor for Enhanced Sustainability in Energy and Environmental Sectors

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Abstract: Superhydrophobic surfaces have attracted the attention of researchers in a range of environmental applications such as self-cleaning, anti-corrosion, anti-fouling, anti-icing, and heat transfer. Superhydrophobicity is typically achieved through low surface energy and high micro to nano-scale surface roughness, allowing reduced contact between the liquid and the surface of solid material. Due to their increased roughness, superhydrophobic surfaces face vulnerability under mechanical stress. This roughness causes high localized pressures, making the surfaces prone to abrasion damage, altering its wettability and reducing durability in harsh environments. In this study, a two-steps methodology is proposed to achieve robustness in superhydrophobic surfaces, making them resistant to mechanical abrasion wear and harsh operating conditions, such as acidic/alkaline environments, sea water, ultraviolet (UV) radiation, and elevated temperatures. Initially, the mechanical robustness is achieved through interconnected armor grids by a single-step laser-induced micro-to-nanoscale texturing. Then, the low surface energy was achieved through silica-based superhydrophobic nanocoating. Inspired by biomimicry architectures such as honeycomb structures, various shapes (hexagonal, triangular, and square) and sizes of grid microstructures with interconnectivity were explored. The grid microstructure, with pockets for nanocoating, serves as protective armor for the superhydrophobic coating, enhancing its abrasion resistance and maintaining its water-repellent properties. The initial water contact angle (WCA) was 168 degrees, and after 1000 sandpaper abrasion cycles, the surface maintained its superhydrophobicity with a dominant WCA above 150 degrees. The effectiveness of these designs was quantitatively assessed through exposure to UV radiation for 30 days, immersion in sea water and harsh chemical environments, and repeated thermal cycling. Our findings reveal the potential of superhydrophobic surfaces for energy and environmentalrelated applications such as enhancement of solar-panel's efficiency through self-cleaning properties. Moreover, the scalable nature of this method opens pathways for widespread application across multiple industries, promising a new standard for durable, energy-efficient, and environmentally resilient surfaces.

F4.3

Electro-magnetic coupling through ion motion in hydrogel

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Faraday's law of induction indicates that an Electro-Motive Force (EMF) can be induced by changing a magnetic field or moving a conductor in a magnetic field. Hydrogels are conductors of ions. This work studies the mechanism of transduction from the input magnetic field to the output voltage of hydrogels. Cyclic magnetic field at different frequencies and amplitudes is applied on hydrogel samples and the induced voltage is measured simultaneously. Besides tests, theoretical analysis is also conducted. Both experimental and theoretical investigations reveal a scaling law between the output voltage amplitude and the input field amplitude and frequency.



Figure 1. (a) Experimental setup. (b) Induced ion current. (c) Comparison between experimental results and theoretical predication.

Poster ABSTRACTS

The *In-situ* Acetylation of Bacterial Cellulose by Using N-Acetyl Glucosamine as an Alternative Carbon Source

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The modification of Bacterial Cellulose (BC) is a highly studied field however in the aim of sustainability and scalability there are often issues with the number of steps required to modify BC, as well as the chemicals used for modification being costly and potentially ecologically damaging. In this study we showcase a one pot method of acetylating BC by replacing the glucose traditionally used in media with Nacetyl Glucosamine (NAG). We demonstrate that this method can produce a mechanically homogenous form of BC with a consistent tensile strength compared to plain BC. The water contact angle was also improved over plain BC with the NAG providing a contact angle of over 90 ° for some samples and retaining a greater contact angle after 1 minute than the plain BC controls. Furthermore, we analysed the metabolic profile of the Komagataeibacter xylinus during the growth cycle of the pellicle to provide information on the mechanism by which NAG is incorporated into the BC. We characterised the material using FTIR, SEM, EDX, and LC/MS of the pellicles to allow us to confidently confirm that the BC had been modified by the incorporation of NAG into the chemical structure of BC. This study demonstrates that a functional one pot modification of BC is possible by modifying the chemical feedstock of *K. xylinus* and that there is potential for further optimisation of this methodology to produce BC with greater functionality.

Integration of Green Hydrogen in the UK Local Bus & Coach Transport System: A Comparative Life Cycle Analysis of Diesel Fossil Fuel and Green Hydrogen Powered Buses

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Abstract

Greenhouse gas (GHG) emissions have profound impacts on the environment and human life. The transportation sector generates the largest share of greenhouse gas emissions. Buses combined with coaches, represented 3% of UK transport emissions and 1% of total mileage in 2019¹. In 2022, the UK local buses' millage was 1.1 billion miles counted for 31,000 buses which 79% of them were diesel powered ². This research provides a comprehensive computational analysis of GHG emissions associated with integrating green hydrogen into UK public and local bus sectors. Herein, we investigated the potential for reducing the greenhouse emissions by replacing 25%, 50% and 100% of diesel buses in the UK by green hydrogen fuel (GHF).



Figure 1. CO_2 emissions savings for 100% conversion of Diesel buses to hydrogen buses. Red, blue and green columns represent Metric tons of CO_2 emitted by using diesel fuelled bus, green hydrogen fuelled buses, and GHG emission savings in four different timescales.

The result in Fig 1. indicates that if 100% of UK local buses converts to green hydrogen powered buses by 2030 the reduced emissions by busses and coaches will be approximately 91.92 % which will contribute into the UK government aim to reduce total GHG emissions by 68% in 2030.

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Droplet impact energy harvester enabled by coplanar reverse electrowetting-ondielectric (CREW)

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Generating energy from liquid droplets, such as ionovoltaics [1] and hydrovoltaic [2] energy harvesting technologies, have become an emerging force in sustainable energy systems. This paper introduces a novel open-top (Fig. 1a) coplanar electrode Reverse Electrowetting on Dielectric (c-REWOD or CREW) setup designed to address inherent challenges in conventional raindrop energy harvesting systems [3]. The CREW configuration offers a unique solution with both energy harvesting electrodes (EHE) and counter electrodes (CE) on the same plane. This enables the REWOD technologies to be adaptable and optimised for droplet impact and subsequent energy conversion, enhancing the efficiency of raindrop energy harvesting [3]. Positioned as an interesting alternative to triboelectric methodologies, the research explores potential applications and scalability of coplanar REWOD systems [4, 5]. The experimental phase of this study focuses on testing deionised water droplets of varying volumes released from a fixed height onto the coplanar reverse electrode testing platform. Test structures (Fig. 1b) designed to have varied EHE:CE area ratio enabled research on the system's performance under different key parameters, such as coating materials and their thicknesses, EHE:CE ratios, droplet composition and dynamics (Fig. 1c), providing valuable insights into its practicality and adaptability. The energy generation per droplet has been examined giving systematic approach in CREW optimisation and application exploitation. The initial results have revealed complex relationship between EHE:CE ratio against instantaneous output power, while also demonstrated valuable insights into the relationship between other design aspects.



Figure 1. (a) Droplet impact on "open-top" reverse electrowetting-on-dielectric energy harvesting device enabled by coplanar electrodes configuration. (b) Test structures with different EHE (purple coloured coated with tantalum pentoxide dielectrics) and CE (grey coloured tantalum metal) electrode area ratios for CREW. (c) High-speed video frame shows droplet impact on the CREW test structure surface.

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Sequential buckling architected graphene aerogel for ultra-sensitive sensor

Abstract No.

041

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Wearable sensors for human motion detection often use reduced graphene aerogels as pressure sensors, but their conventional production limits their effectiveness¹. In this study, a unique CCS-rGO (crosslikned chitosan-reduced graphene oxide) aerogel with a special microstructure is created using freeze-casting and thermal post-buckling which only needs 180°C for 3h. Through this method, the energy consumption is obviously decreased compared with the conventional reduced graphene aerogel achieving for similar properties². The aerogel's structure allows it to withstand compression without collapsing, recovering its shape after unloading. It also exhibits excellent fatigue resistance after 20000 cycles. Leveraging these properties, CCS-rGO aerogels are employed as piezoresistive pressure sensors for detecting human motion signals. Demonstrations and an analytical model further showcase the effectiveness of these aerogels in pressure sensor applications.



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Innovative Indirect Evaporative Coolers Design Framework: A Way Forward to Energy Efficiency and Net Zero

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The last few decades have seen a notable increase in the demand for cooling. At the moment, energyintensive mechanical vapor compression chillers that use hazardous chemical refrigerants dominate the cooling industry. As a result, the creation of novel, environmentally friendly cooling technologies is the present emphasis of cooling research. This is where indirect evaporative coolers, with their high energy efficiency, cheap cost, water-based sustainable operation, and benign emissions, have shown great promise, especially in hot, dry conditions. Due to various design issues, some systems are still in the development stage and have not yet reached full commercialization. In this study, a novel indirect evaporative cooler is designed, built, and tested experimentally. The creation of the heat transfer coefficient correlation for the system's commercial-scale design and growth is the study's primary focus. This is because the previous correlation that was available was based on the basic airflow between parallel plates assumption and neglected to account for the system's evaporative potential, which led to an under- or overestimation of the heat transfer characteristics. The suggested system was able to accomplish a 20 °C temperature decrease, a cooling capacity of about 180 W, and an overall heat transfer coefficient of up to 30 W/m2K, according to the data. Additionally, the paper offers an experiment-regression-based heat transfer coefficient correlation that adequately accounts for the influence of airflow rate ratio and external air temperature, two factors that are crucial for evaporative cooler design. The suggested correlation shows a good degree of agreement $(\pm 5\%)$ with empirical data, so rendering it appropriate for the design of IEC systems under various operating conditions in the future.

Sustainable Wood-based Functional Structural Materials

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We used an innovative approach involving hot pressing, low energy consumption, and no adhesive to transform wood into a natural sustainable fiber-based bio-composite for structural and furniture applications. Analyses showed strong internal bonding through mechanical "nail-like" nano substances, hydrogen, and ester and ether bonds. The bio-composite encompasses a 10-fold increase in internal bonding strength with improved water resistance, fire safety, and environmental friendly properties compared to existing furniture materials using hazardous formaldehyde-based adhesives. Compared to natural wood material, this new bio-composite have improved fire and water resistance while there is no need for toxic adhesives (mostly made from formaldehyde-based resin), easing the concern of harmful formaldehyde-based VOC emission and ensuring better indoor air quality. This surpass existing structural and furniture materials made by synthetic adhesives. Interestingly, our approach can 100% convert discarded wood biomass into this bio-composite, representing a potentially cost reduction alternative with high revenue. Te underlying fragment riveting and cell collapse binding are obviously a new technology approach which offers an economically and sustainable high-performance bio-composite that provides solutions to structural and furniture materials bound with synthetic adhesives.



Poster story: A high-performance and sustainable structural functional material has been developed from natural pinewood, enabled by the unique ionic bond. The obtained material shows good water resistance, thermal conductivity, thermal stability, UV resistance, corrosion resistance and antibacterial properties. This material has promising applications in waterproof enclosure structure, underfloor heating, UV resistant protective cover, and anti-corrosion materials, etc.

A Novel Adsorbent Based Atmospheric Water Generator System for Net Zero

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The high rate of GDP growth is expected to drive up water demand by over 200%, 140%, and 130% for industry, power generation, and home sector consumption, respectively. It will increase the global water demand by nearly 55% by 2050. Therefore, 40% of the world's population will live below the water scarcity threshold due to current consumption trends. One of the most workable and sensible ways to close the supply-demand mismatch is through seawater desalination. Currently, 150 nations are home to over 19,000 desalination units, producing about 38 billion m3 annually. However, this solution is only viable for the places with accessible seawater supply. Meanwhile, centralized approaches for water generation are becoming more popular because of standalone supply at point of utility. Atmospheric Water Generation (AWG) is the best alternative for producing fresh water. Many modern technologies have been introduced for this application. For instance liquid desiccants AWG systems produced 0.63 to 1.0 kg/m/d of water. Metal-organic frameworks (MOFs) have shown excellent hydrophilicity, structural integrity, and tailorable structures to provide water in high and low humidity areas. MOFs yielded maximum adsorption uptakes at 25 °C of 0.3 to 0.5 g/g. MOF-801 showed an excellent water production of 0.2-0.3 L/kg/d at 5%-40% RH and 20-40 °C. MOF-303 delivered ~0.7 L/kg/d at 10% RH and 27 oC. Cr-soc-MOF-1 and MIL-101(Cr) resulted in maximum adsorption uptakes i.e., 1.9 g/g and 1.4 g/g, respectively. However, all these systems are prone to productivity variation with changing outdoor air conditions such as temperature and humidity. We proposed a novel AWG technology based on silica gel adsorbent with retrofitted arrangement of the components that is insensitive to the outdoor air conditions. Our proposed system can achieve up to 20 L/d with 20% less energy consumption than the conventional systems. Moreover, the system can also be opera

Biomimetic Spinning of Multil-structure Fibers via Bubble Separation for Hydrovoltaic Electricity Generation_

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Functional flexible fiber materials have diverse applications in electronic fabrics, energy, and various fields ^{1, 2}. Current technologies for fabricating single-fiber materials include dry/wet spinning^{3, 4}, microfluidic spinning⁵, thermal drawing⁶, and direct printing⁷. While excelling in functional fiber production, these methods encounter limitations in diversification. In nature, organisms like spiders and silkworms efficiently modify fiber morphology for specific purposes (Figure 1a), predation and concealment being notable examples, through a highly effective and straightforward fabrication process⁸.

Inspired by the multimodal spinning abilities of spider silk glands, we developed a bubble-assisted spinning technique (Figure 1b). This method enables the creation of diverse fiber morphologies, such as gourd shells⁹, *N. alata* rosettes¹⁰, and spindle knitting¹¹, without altering the spinneret. These fibers exhibit efficient water collection and transfer capabilities. Additionally, fibers produced with organic polymer-intercalated two-dimensional (2D) materials demonstrate proton transfer between layers in humid conditions. Due to the synergistic interaction between biomimetic structures and 2D materials, the method yields functional soft fibers with humidity-electric conversion and humidity sensing capabilities.

This innovative fabrication method provides a cost-effective solution for producing multifunctional flexible fiber materials, promising advancements in the development and innovative applications of materials in the field of fiber electronics.



Figure 1. Design of biomimetic spinning of multil-structure Fibers.

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A biocompatible, thin, and wet-adhesive zinc-ion hybrid supercapacitor as an implantable power source

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As societal development progresses, the aging population continues to rise, leading to a surge in healthrelated issues. The escalating prevalence of neurological and cardiovascular diseases has underscored the urgent need for implantable electronic medical devices, which have emerged as a significant component of contemporary clinical medicine. The latest generation of these devices boasts flexibility and convenience in both form and function, positioning them as a focal point for research and development globally. Notable examples include electronic pacemakers for cardiac arrhythmia treatment ^[1], deep brain stimulators for Alzheimer's disease management ^[2], vagus nerve stimulators for epilepsy therapy ^[3], and cochlear implants ^[4]. These devices significantly enhance patient outcomes, curtail healthcare expenses, elevate quality of life, and extend patient lifespan. Nonetheless, the stable and uninterrupted functioning of these implantable electronic medical devices is contingent upon the utilization of power supplies characterized by high reliability, elevated energy density, and minimal toxicity. Here, we propose a thin, flexible, and wetadhesive zinc-ion hybrid supercapacitor (ZHSC) as an implantable power source with superior biocompatibility. This work provides an example for the design and fabrication of biocompatible, thin, and wet-adhesive implantable energy storage devices with high performance.



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Synthesis of CNF/EP composite for corrosion resistance application on carbon steel

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Improving the barrier potential and anticorrosion properties of coatings requires reducing flaws and increasing the interfacial compatibility of nanoparticles and resins. These variables further limit the use of carbon nanofiber in epoxy organic coatings. We present the creation of a CNF on carbon steel using a controlled pyrolysis technique and coating it with aqueous epoxy resin to improve anti-corrosion performance. For the evaluation of structure, wettability, and molecular compositions, FTIR, SEM, water contact angle measurement, Raman spectra, and XPS are used. The study employed Electrochemical impedance spectroscopy (EIS) and PDP to assess the effectiveness of CNF/EP nanocomposite in preventing corrosion on a steel substrate. The current study identified CNF/EP as a viable material for innovative coatings designed to prevent chloride induced corrosion of carbon steel.

ASSET-LIABILITY MANAGEMENT AND BANK EARNINGS OF COMMERCIAL BANKS IN NIGERIA

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Earnings have become one of the major reasons banks are still in existence. Achieving targeted earning by banks has become major challenge. This challenge has created mis-match of assets-liabilities which in turn led to decline in bank earnings in Nigeria. Objective of the study focused on effect of Asset-Liability Management (ALM) on bank earning among commercial banks in Nigeria. Fixed panel regression and System GMM techniques with *expost facto* research design were employed for the period of 2010-2021. Finding revealed that ALM components influenced bank earnings. Thus, the study suggested that bank top management should give more sound priority to both ALM policies and bank size or bank total asset and also ensure no assets-liabilities mis-match so as to achieved sound bank earning among banks in Nigeria.

BIOGAS PRODUCTION USING ANAEROBIC DIGESTION OF AGRICULTURAL VEGETABLE (CABBAGE AND SPINACH) RESIDUES

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Microbial energy technologies employ microorganisms through the breakdown of organic materials to transform chemical energy in biomass into energy-bearing fuels. Biogas is a product of fermentation from biodegradable materials which serves as profitable means of reducing or even eliminating the menace and nuisance of urban wastes while serving as a reliable source of renewable energy. This study used Agricultural residues of spinach, cabbage and cow dung as substrates through several interdependent, complex sequential and parallel biological reactions in the absence of oxygen. Seven treatments were prepared while temperature, pH, and proximate compositions (moisture, ash content, volatile compounds, fixed carbon, nitrogen and crude fibre) were recorded at 24 hours intervals for 30 days. The results indicate rapid increasing gas production within the first ten days with the exception of a treatment that comprised mixture of cabbage and cow-dung. The highest volume of biogas (1346.552 cm³) was obtained from the treatment of cow dung followed by mixture of the three substrates with 1232.759 cm³ biogas composition. All components of the biogas were confirmed using the GC-MS analyses. Temperature values above 40°C were noticed throughout the experiments while pH values were entirely acidic. All the bacteria isolates obtained belonged to the categorise of Staphylococcus, Bacillus and Proteus species. This shows vegetable waste can be utilized by microorganisms for sufficient biogas production. Utilization of such substrates could be as a result of accessibility by the identified bacteria. Hence, the species played a vital role in biogas production from vegetable wastes.

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Water Quality Modeling Using Artificial Neural Network at the Dead-End Sections of Drinking Water Distribution System

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Despite efforts in treating water in water distribution systems, water borne disease outbreaks persist as a result of undergoing factors within the treatment tank, one of which is the water condition at the dead-end section. Existing models have addressed these problems in the mains and distribution, but that of dead end is still lagging. Therefore, this research seeks to address issue of water deterioration at the dead-end section of water distribution system of Abuja, Federal Capital territory of Nigeria. The Artificial Neural Network (ANN) model was deployed, for its ability to accurately model data of both short and long duration so as to establish dependability of the governing water quality parameters. An 8:9:1 ANN Architecture with 70:15:15 random data distribution for training, testing and validation of ANN I, ANN II and ANN III being the models for Rainy, Dry and Combined Seasons data respectively was adopted and error was minimized using the feed forward techniques MLBP Algorithm (back-propagation technique). From results, ANN I model with Output = 0.68 performed better than the other two (ANN II and ANN III). Performance and reliability, when quality was simulated at selected Dead-Ends of Gudu Water Distribution System (WDS) with EPANET, yielded 92.36% efficiency, R2 value of 0.81 and 0.00092 performances which are high and better than those of obtained from multiple regression. This suggests that the quantity of disinfectants for the rainy season data within the dead-end sections is more functional and reliable within the WDS than those of the other two seasonal combinations.



Fig. 1: Multilayer Perceptron Neural Network for the Chosen Water Quality Parameters

AFLATOXINS IN FOOD PRODUCTS CONSUMED IN THE KINGDOM OF SAUDI ARABIA: A PRELIMINARY DIETARY RISK ASSESSMENT

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Aflatoxins (AFs) are hepatotoxic, mutagenic, genotoxic, and immunosuppressive toxins. Several food commodities consumed in the Kingdom of Saudi Arabia (KSA) are susceptible to AF contamination because of improper storage practices and the warm and humid climate of the country. Therefore, the occurrence of AFs in 2388 food samples was measured and the estimated daily intake (EDI) of AFs in Saudi adults was assessed. The risks of AFB₁ exposure were characterized using the margin of exposure (MoE) approach and by estimating the number of possible hepatocellular carcinoma (HCC) cases in the KSA. The results revealed that 12.1% of the analyzed samples were contaminated with AFs and the highest concentration of total AFs was observed in the nut and seed group. The mean EDI of AFB₁ was estimated to be 0.21 and 0.55 ng/kg body weight (bw)/day for the lower bound (LB) and upper bound (UB) scenarios, respectively. The MoEs were estimated to be 1902.4 and 722.1, while the estimated liver cancer risk ranged from 0.002 to 0.008 cancer cases/year/100,000 persons. Based on the study's findings, contamination with AFs in the KSA is low; however, AFs are considered potent genotoxic contaminants, and therefore, exposure through food should be kept as low as possible.

BIOGRAPHY

Jumanah Alamir has her expertise in food safety and passion in improving the human health and wellbeing. She conducted scientific reports and research projects related to food safety and risk assessment including natural toxins, environmental contaminants. She participated in a several working teams in designing and analyzing data of a yearly National Food Monitoring Program conducted in cooperation with multiple governmental bodies. Additionally, she is an expert in reviewing and updating technical specifications and regulations of chemical hazards in food. She is currently a member in the following International Scientific Committees; The Codex Committee on Residues of Veterinary Drugs in Foods as well as ISO/TC 34/SC 7 Spices, Culinary Herbs and Condiments Committee.

Next-Generation Technologies and Sustainable Practices in Offshore Oil and Gas Exploration: A Roadmap for Environmental Stewardship and Industry Resilience

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The surging demand for oil and gas products, coupled with escalating environmental threats from industry activities, necessitates a paradigm shift. It is imperative to bridge the widening gap between technological advancement and regulatory enforcement to ensure the sustainable future of oil and gas exploration, particularly in the face of growing challenges in emissions control due to environmental factors. This paper introduces a groundbreaking approach that leverages next-generation technologies and cutting-edge sustainable practices to usher in a new era of environmental responsibility within the oil and gas sector. It not only identifies emerging trends but also outlines the essential conditions for the widespread adoption of these innovative solutions. At the core of this paradigm shift is a meticulously designed architecture that seamlessly integrates next-generation technologies and sustainable practices, aiming to revolutionize oil and gas exploration by making it not just efficient but inherently environmentally friendly and safe. What sets this proposed model apart is its novel combination of advanced technologies and sustainable practices, promising a transformative impact on the entire oil and gas industry. The proposed architecture incorporates advanced sensor technologies and artificial intelligence for real-time monitoring of emissions. This ensures precision in tracking and controlling environmental impact, addressing a critical challenge in the industry. A novel aspect of the model involves the implementation of closed loop recycling processes, minimizing waste generation during oil and gas extraction. This sustainable practice contributes to environmental conservation and resource efficiency. Unlike traditional approaches, the model integrates renewable energy sources, such as solar and wind, into the extraction process. This not only reduces reliance on fossil fuels but also contributes to a more sustainable and eco-friendly operation. The model incorporates an adaptive risk management framework, utilizing real-time data and predictive analytics to assess and mitigate environmental risks dynamically. This proactive approach enhances safety measures and aligns with evolving regulatory standards. By meeting the evolving requirements of new applications, the model stands as a testament to its novelty, efficiency, scalability, and its inherent suitability for the future of oil and gas extraction.

Synthesis of Novel Activated Carbons Derived from Pig Fur Biowaste for Cadmium Adsorption in Wastewater

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This research investigates the viability of pig fur biowaste in the synthesis of activated carbons (ACs) for cadmium adsorption in wastewater. In two different activation methods–in-situ and ex-situ activations–the effect of impregnation ratio, carbonization temperature, and time on the cadmium adsorption capacities of the two resulting ACs was investigated using the central composite design (CCD) of the response surface methodology (RSM). For the in-situ activation, the optimum conditions obtained were 691 °C, 175.11 min, and 1.784 g/g for carbonization temperature, time, and impregnation ratio, respectively, while for the exsitu activation, the optimum conditions were 468.8 °C, 80.81 min, and 2.915 g/g. Although the different optimum conditions produced highly porous ACs with heterogeneous surfaces, the ex-situ-derived AC had a higher cadmium adsorption capacity of 92.85%, while the in-situ-derived AC had 90.355%. The ex-situ activation route is therefore a better activation method for this novel biomass precursor

Optimized microstructure for enhanced properties of novel ecofriendly green plants wastes hybridized epoxy resin eco-composites

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The utilization of eco-friendly green plant waste materials as reinforcing agents in epoxy resin-based composites represents a sustainable and environmentally responsible approach to material development. The primary objective of this research is to explore the reinforcing characteristics of synthesized Mangifera indica shell nanoparticulates (MISNp)/calcium oxide (CaO) hybrid on the thermal, flexural, and mechanical properties of epoxy resin- based eco-composite. The MISNp was synthesised using a sol-gel technique. The MISNp/calcium oxide hybrid were in the ratio 0.2:0.1, 0.2:0.2, 0.2:0.3, 0.2:0.4, and 0.2:0.5 by weight. The eco-composites were fabricated using hand-layup technique and cured at room temperature for 8 days. The thermal behavior of the MISNp and epoxy resin based eco-composites was examined using Thermogravimetric analysis (TGA). The flexural, thermal conductivity and mechanical properties of the developed eco-composites were also investigated. The microstructure evolution and Phase compositions of the eco-composites were analyzed using Optical Microscope, Scanning Electron Microscope (SEM), X-ray Diffractometer (XRD), and Energy Dispersive Spectroscopy (EDS). The functional groups present in the MISNp were also examined using Fourier Transform Infra-red (FTIR) spectroscopy.



Figure 1: Mangifera indica particulate

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EFFECT OF FIRING TEMPERATURE ON THE REFRACTORY PROPERTIES OF MGBOM CLAY

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The effect of firing temperatures on the refractory properties of Mgbom clay deposit was established. The clay sample was collected from the deposit and was processed. The chemical and mineralogical analyses were done using X-ray fluoresce and X-ray diffraction respectively. The sample was processed, molded, dried and fired at different temperature of 9000C, 11000C and 12000C. The refractory properties were tested based on ASTM standards. Results obtained show that Mgbom clay has 28% alumina and 58.6% silica, 8.68% iron oxide, 1.5% potassium oxide and other oxides in trace quantities. Mineralogical phase analysis confirmed the presence of quartz, kaoline and rutile in the clay structure. Hence, Mgbom clay qualifies for fire clay. At the various respective firing temperatures of 9000C, 11000C and 12000C, the values of the refractory properties such as linear shrinkage, water absorption, apparent porosity, bulk density, modulus of rupture, thermal shock resistance and refractoriness were obtained as (4.09 - 7.27%), (8.49 - 0.51%), (15.65 - 1.01%), (1.84 - 1.99g/cm3), (27.26 - 39.28N/mm2), (21 - 28cycles) and (1250 - 16500C) respectively. It was found from the results that firing temperature showed a linear relationship with the clay properties and that clay's optimum properties are obtainable at the firing temperature above 11000C. Therefore, it was recommended that firing temperature above 11000C should be used as appropriate temperature for firing Mgbom clay base materials.
Simulation of polymer membranes for hydrogen production using machine learned interatomic forcefield

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With the need for transition to net zero, new methods of generating and storing energy will be paramount. Hydrogen is a promising candidate for the storage of renewable energy. This is due to its high energy density and the ability to readily convert stored hydrogen to electricity via fuel cells. Proton exchange membrane water electrolysers (PEMWEs) are very promising for green hydrogen production given their technological maturity and high output hydrogen purity with lower power consumption compared to other WEs that are currently commercially available¹.

Operation of PEMWE at high temperature (100–200 °C) will allow greater hydrogen production due to higher reaction kinetics. This is also beneficial as current typical low temperature (40–80 °C) PEM-WEs and PEM-fuel cells require expensive noble metal catalysts². These catalysts make up a large proportion of the cost of the device yet are difficult to replace due to the highly acidic environment of the PEM-WE². At higher temperature, the same overall performance can be obtained with a cheaper catalyst. However, due to fast degradation of current materials (perfluoroakyl sulfonic acid) at high temperature, new membrane materials are necessary for this approach³.

The polybenzimidazole (PBI) membrane is a promising candidate for use in high temperature PEM-WEs due to its stability in higher temperature environments compared to other membranes³. There have been modifications to PBI membranes to improve their ionic conductivity and durability using both experimental and computational studies⁴. Using molecular dynamics simulations based on a newly developed machine-learned forcefield (the MACE module)⁵, existing PBI polymer membranes are simulated to investigate the characteristic of the material under different temperature and acid doping level. This MACE machine learning based model is being used due to consideration of accuracy, simulation time compared to classical molecular dynamics and density functional theory method. MACE also can simulate chemical bonds breaking and forming for Grotthus method transport and during the degradation process. Values such as proton conductivity and mechanical strength are calculated and the chemical stability of the membrane polymers is established. Ultimately, the proposed method will be used to optimise and innovate the membrane material design.

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Excellent Reaction Kinetics and Low-Temperature Adaptability of Zinc Batteries Enabled by Water- Acetamide Symbiotic Solvation Sheath

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While having a high activity, intrinsic safety, and cost-effectiveness, rechargeable aqueous zinc batteries are also known to cause corrosion and a rapid hydrogen evolution reaction. ¹⁻³ Considering the fact that eutectic electrolytes can successfully resolve these problems, their high viscosity significantly decreases Zn^{2+} ion mobility and results in poor temperature adaptation. ⁴⁻⁶ Here, the $Zn(H_2O)_3(ace)(BF_4)_2$ is created by infusing acetamide molecules with Lewis base and hydrogen bond donors into a solvated shell of $Zn[(H_2O)_6]^{2+}$. In comparison with 1ace-0H₂O, which has a viscosity of 995.6 Pa s, a freezing point of 12 °C, and an ionic conductivity of 4.04 mS cm⁻¹, 1ace-1H₂O has a viscosity of 0.032 Pa s, a significantly lower freezing point of -45 °C, and an enhanced ionic conductivity of 9.56 mS cm⁻¹. Additionally, a uniform and dense ZnCO₃/ZnF₂-rich organic/inorganic hybrid solid electrolyte interface (SEI) is formed to isolate direct contact between H₂O and Zn anode. Benefiting from these synergistic effect of unique solvation structure of $Zn(H_2O)_3(ace)(BF_4)_2$ and the formation of SEI layer, the Zn||Zn cells can cycle more than 1300 hours at 1 mA cm⁻², and the Zn||Cu operates over 1800 cycles with an average Coulomb efficiency (CE) of ~99.8%. More notably, the Zn PANI exhibits ultra-stable durability over 8500 cycles with a high specific capacity of 99.8 mAh g⁻¹ at 5 Å g⁻¹ at room temperature and stable operation at low temperature of -40 °C, with a capacity of 66.8 mAh g⁻¹ delivered. This work offers new insights for the development of novel electrolytes to improve the reversibility of Zn anodes. The authors are grateful for the financial support from a grant from the Hong Kong Research Grants Council (RGC, Project CityU 11215121). This research was also supported by National Natural Science Foundation of China (52202299) and the Hong Kong Polytechnic University (WS19).



Schematic illustration of Zn anode/electrolyte interfaces and interfacial reaction processes between electrolytes and the Zn anode and hydrogen bond reconstruction with acetamide.

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

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The doping and anchoring of single-metal atoms into graphdiynes (GDYs) can tune their electronic structure and broaden the usage. Herein, metal elements as a new functional units can be introduced into the frameworks of GDYs via metal-alkyne bonds to afford novel metallated GYs (MGYs). However, related research work is still in its infancy and their large-area and free-standing nanosheets were first isolated for use in the optical devices and catalysis by us in 2021. The novel MGYs has been designed and synthesized with homo- or hetero-metallic skeleton via the facile bottom-up method, which integrates the advantages of both metal centers and graphyne frameworks. The propensity of d₁₀ Hg(II)-, d₈ Ni(II)-, Pd(II)- and Pt(II)-(PR_3)₂ (R = alkyl chain) units to form a moiety with alkynyl units makes them attractive building blocks for 2D organometallic functional materials. Both few-layer and multi-layer 2D nanosheets can be generated depending on the types of interface-assisted (i.e. liquid/liquid and gas/liquid) approaches and their bulks can be prepared by the one-pot method. The ligand structures and electronic properties can be easily adjusted in terms of the spacer length between the ethynyl unit and central core, central chromophore as well as the number of coordination sites. Therefore, the 2D nanosheets with different topological structures, pore sizes, surface areas and advanced functionalities can be prepared by using different monomers with diverse electronic, optical and catalytic properties. The relationship between the performance of MGYs and their well-defined nanostructures will be elucidated, with a major focus on studying the effects of transition metals and ligands in activating their optical and catalytic properties. The properties and catalytic performance can be fine-tuned through chemical modification of the chromophores. The proposed work can produce a new class of 2D carbon-rich materials and provide a design concept for developing efficient nonlinear optical materials and photo-/electro-catalysts.

Constructing and Advancing Robust Electrodes for Optimised Hydrogen Production Under Fluctuating Power Supply

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Hydrogen production through water electrolysis is pivotal in steering the global energy framework towards sustainability. Integrating this process with fluctuating renewable energy sources, such as wind power, presents a promising avenue. However, the inherent intermittency of these sources can adversely affect the operational stability and longevity of the electrolytic cell electrodes.

This study rigorously investigates the impact of fluctuating voltage on the performance and durability of these electrodes. It aims to dissect the underlying mechanisms of electrode degradation under variable power conditions and devise strategies to mitigate these detrimental effects. Through meticulous examination and innovative methodologies, this research intends to offer profound insights into optimising electrolytic hydrogen production systems, especially those powered by intermittent renewable sources.

The anticipated findings are expected to be instrumental in enhancing the efficiency and sustainability of hydrogen production, thereby significantly propelling the hydrogen economy forward. This research not only addresses a crucial technological bottleneck but also paves the way for more resilient and sustainable energy systems in the future.

Thin, Stable, and Flexible Lithium Metal Anodes for High-Performance Lithium Metal Batteries

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Equipping thin (\leq 50 µm) lithium metal anodes (LMAs) is essential to realize high-energy-density batteries.^[1] However, the unsatisfactory cycling stability of thin LMAs,^[2, 3] especially at high depth of discharge (DOD), is a long-standing bottleneck in the battery field. Meanwhile, the limited mechanical flexibility of thin LMAs remains a huge challenge in realizing the next-generation flexible lithium batteries. Here, we report two novel strategies to develop thin, stable, and flexible LMAs for long-lifespan, energy-dense, and highly-flexible lithium metal batteries (LMBs).

A promising thin LMA is realized through selective wetting of molten Li on a Janus conductive textile. This textile host, comprising a lithiophobic nickel side and a lithiophilic nickel antimonide side, shows Janus Li wettability. When contacting the molten Li, only the Li-affinitive side of the textile framework is coated with a thin Li layer (~50 μ m), resulting in the distinctive Janus Li-textile anode (Figure 1a). Importantly, the favorable upper buffering room of the Janus Li-textile anode enables itself with record-prolonged cycling stability (3,000 h operation lifespans at 75% DOD) and impressive mechanical flexibility (folding for 200 times).

A thinner Li metal layer (~40 μ m) assisted with two ultralight fabrics is further proposed to pursue the higher energy density. Enabled by one-step mechanical rolling, the sandwiched Li (SW Li) is successfully developed (Figure 1b). The support of fabric layers can dissipate the stress concentration and prevent rampant surface depositions, thus endowing the SW Li with superior flexibility (1.5 mm bending radius for 10,000 times) and outstanding cyclability (91% capacity retention after 500 cycles). Meanwhile, the flexible SW Li battery realizes a high energy density of >300 Wh kg⁻¹, showing great promise in the next-generation advanced LMBs.



Figure 1. The scheme illustration of (a) Janus Li-textile anode and (b) SW Li.

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In Situ Constructing Weakly Solvating Polyether Electrolytes with Excellent Interfacial Compatibility for High-Voltage Flexible Quasi-Solid-State Lithium Batteries

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Quasi-solid-state electrolyte (QSSE) with high ionic conductivity and excellent interfacial compatibility is required for high-voltage lithium metal batteries (LMBs) to improve energy density and operational safety. Here, we report a QSSE with contact ion pairs (CIP), and ion aggregates (AGG) solvation structures by controlling the concentrations of plasticizers, which improves the stability of both Li anode and high voltage cathode by generating inorganic LiF-rich interphases. Finally, the QSSE exhibits high ionic conductivity at room temperature (5.0×10^{-4} S cm⁻¹), widely electrochemical window (4.8 V), and high Li plating/striping coulombic efficiencies (98.8 % and 98.5 % after 200 cycles at 0.5 mA h cm⁻² and 1.0 mA h cm⁻², respectively). The detailed composition and protection mechanism of anion-derived cathode solid interface (CEI) was investigated in detail with Cryo-TEM, which reveals that CEI with continuous inorganic components can improve the oxidative stability of QSSE. Our QSSE enables LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂//Li cell with long cycling stability (100 cycles) under high area capacity (4 mAh cm⁻²). This work provides an effective pathway toward QSSE for high-voltage LMBs.

Advanced Leading Edge Protection System based on Machine Learning and AI

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NET ZERO is a vital goal in combating climate change. It involves balancing greenhouse gas emissions by removing an equivalent amount from the atmosphere. This transition requires renewable energy sources like wind power to achieve a sustainable future. Wind turbine blades are exposed to precipitation that occurs in a variety of forms and myriad abrasive airborne particles that can, over time, erode their surfaces, particularly at the leading edge. These airborne particles can cause significant blade erosion damage that reduces aerodynamic performance and energy capture. Solving the problem of leadingedge erosion (LEE) requires a comprehensive approach involving various disciplines such as aerodynamics, fluid mechanics, and materials science. Intuitively, adding a protective layer formed by tough material can help leading-edge against erosion. In the past, research on LEE protective materials was primarily focused on developing new materials, new test methods and modelling performance from test to turbine, and has not achieved significant breakthroughs especially for the former and latter. However, with the development of AI and machine learning, a greater opportunity has emerged. The data driven methods, such as regression analysis, will be used to model the performance data, the raw materials, and the production conditions of the protective materials of wind turbine blades. The linkage between the performance and related conditions will be automatically established by using machine learning algorithms. The accuracy of the model will be validated by multiple iterative analyses.

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Robust, Transparent and Multifunctional Polyurethane Containing Ionic Liquids

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The preparation of functional polyurethane elastomers is a hot subject at present, the development of polyurethane materials with the functionality is important for practical applications: however, this remains a substantial challenge. In this work, a kind of ionic polyurethane urea elastomers were prepared via the chemical incorporation of ionic liquids and silane coupling agents. In contrast to conventional polyurethane, this ionic polyurethane exhibited superior mechanical strength and optical transparency. The enriched fluorine-containing anion group and siloxane cross-linked structure contribute to enhanced hydrophobic properties and chemical solvent resistance. In addition, ionic liquids endow polyurethanes impressive high dielectric constants and high AC conductivity. At the same time, the cations in the ionic liquid are existed in the long chain structure, while the anions are dissociative, this difference allows ionic polyurethanes to deform under electric field drive, and surprisingly, this electric field drive can be allowed to be carried out at low voltages, with a bending driving force output of 0.7Pa at only 500V voltage. These multifunctional ionic PU elastomers offer great potential for the design and preparation of flexible materials with electrical sensing ability.



Fig. Synthesis and properties (a-d) of the PU containing ionic liquids

This work was supported by the National Natural Science Foundation of China (No. 51703193), Hebei Natural Science Foundation (No. E2021203047). Z. Zhang was supported by the CSC program.

Combinational Data-driven Innovation of Ecofriendly Transparent Solar Heat Control Coating for Green Buildings

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Transparent solar heat control coating (TSHCc) is an attractive option for efficient green building to minimize energy consumption and improve indoor living comfort owing to their optical properties of modulating sunlight. However, the complete blocking of the entire NIR spectrum has not yet been realized by the coating technology, and the coating development process remains time-consuming and labor-intensive.

Artificial intelligence technologies open a perspective for efficient TSHC coating development at low cost by accomplishing several basic tasks: predicting the transmittance spectrum of unknown materials based on previous observations, predicting the solar heat control performance, and implementing a feedback from performance to coating preparation. To effectively improve the performance of solar heat control coating for green building, we propose a data-driven combinatory strategy to develop the coating composed of multiple nanoparticles for broadband NIR blocking while maintaining high visible transmittance.

Three types of nanoparticles, namely cesium tungsten oxide (CWO), antinomy tin oxide (ATO), and indium tin oxide (ITO), are chosen to prepare a TSHC coating aiming for an ideal performance of 70% visible transmittance and 100% NIR blocking. The neural network model, trained by 108 real experimental datasets, is capable of precisely predicting the transmittance spectrum of the coating based on the concentrations of multiple nanoparticles and inversely designing nanoparticle concentrations based on the desired transmittance spectrum in a sample space of 726 samples, thus significantly reducing the development cost and time. The results demonstrate that the optimized TSHC coating has a visible light transmittance of 70% and a near-infrared blocking rate of 96%. Its light to solar gain reaches as high as 1.4, indicating strong spectral selectivity, which is the highest value reported for TSHC coatings to date.



Figure. Data-driven combinatory development of TSHC coating

Manufacturing Lithium-ion Battery by Electrophoretic Deposition

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Electrophoretic deposition (EPD) is a well-established industrial production process for surface coatings. It is currently finding increasing academic and commercial interest for lithium-ion battery manufacture. Progressing EPD to the next stage requires researcher to move beyond simple demonstrations of the process. This poster will showcase our approaches of moving EPD a step closer to factory. Full-cell LIB in which anode and cathode are manufactured by EPD will be shown. Our learnings about investigations compatible with industry scalability will be shown including:

- Electrolyte chemistry formulation for electrode manufacture
- EPD processes to manufacture battery electrode
- Process control and optimization for coating thickness and mass loading
- Technology comparison with slurry casting
- Scaling research testing coin cells to pouch cells
- Ease of manufacture with porous current collectors for high power

Exemplary battery chemistries will be reported, showing the scientific development of EPD with anode lithium titanate(LTO) and cathode lithium iron phosphate(LFP), in related liquid electrolyte and solid-state lithium devices. This presentation will share the practical performance of EPD electrodes has outperformed slurry casting in various categories including lower resistances, more extractable capacity, high power capability and stable cycling robustness. Challenges of EPD will be listed.

It is hopeful that this poster will act as a springboard for the development of future collaborative R&D with the communities of electrochemical engineering, and intends to influence research innovation of EPD technology for lithium-ion battery.

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Performance Monitoring of Reinforced Concrete Anaerobic Digester Tank using Non-Destructive Test Methods

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The cost of replacing civil assets can be expensive and ultimately results in increased costs to customers (Reddy, et al., 2018). Major challenges faced by civil asset operators include moving to more efficient predictive maintenance regimes and understanding the processes through which assets fail so that they can be monitored, and end of life assessed and predicted more accurately (Omar, et al., 2019).

This project is focused on reinforced wastewater concrete tank structures used extensively by wastewater companies. Durability is the characteristic of a reinforced concrete structure to carry out its intended purposes while maintaining the necessary strength and serviceability during the anticipated service life (Neville, 2001). The major durability problems in reinforced wastewater concrete tank structures are caused by the cyclic loading and unloading of the structure (Hamdoon, 2012), unsuitable choice of construction techniques and materials (Meyer & Bennett, 2002) and environmental conditions particularly the varying temperature conditions in inside and outside of the tank (Nabil F. Grace, et al., 2021). These conditions lead to propagation of cracks, seepage, and the potential for corrosion of the steel reinforcement in the structure (Bohni, 2005). This project will characterise the surface and internal cracked state of wastewater tank assets using non-destructive tools. The results will utilise the data gathered from the tests to develop an asset deterioration model to prognostically determine the requirement for maintenance interventions and to forecast the remaining useful life of reinforced concrete tanks.

Enhancement of Hydrogen Evolution Reaction Performance of 3D Pyrolytic Carbon derived from 3D Printing

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Considering its clean and fully recyclable nature, hydrogen generated through water electrolysis is a potential alternative to fossil fuels. However, the ability of hydrogen to hold the next-generation fuel capability is affected by the unaffordability of the water electrolyzer systems and practical-level electrochemical performance. Moreover, the oxygen evolution reaction remains enigmatic in the overall water-splitting reaction.1 Recently 3D printing additive manufacturing technology has been explored for electrochemical applications including hydrogen evolution.2 This work involves the fabrication of polymer template-based electrode using stereolithography (SLA). The main novelty of the work lies in using a Rod-Connected Diamond-based geometry, i.e. whose topology is similar to that of an atomic diamond crystal, where bonds between atoms are represented by cylinders. According to literature, the electrode activity can be improved by increasing and optimising the active surface area and the intrinsic activity of the material. Hence printable 3D polymer structures with different filling fractions can be designed and subsequently analysed for material and electrochemical performance. The post-processing involves carbonizing the polymer template through thermal decomposition followed by nickel electroplating and chemical vapour deposition of g-C₃N₄ with the purpose of obtaining nitrogen-carbon-nickel hybrid electrode- electrocatalyst system. The electrochemical performance of the electrocatalyst has been analysed via techniques such as voltammetry, electrochemical impedance spectroscopy and chronoamperometry. The analysis revealed that the intrinsic activity of the pyrolytic 3D carbon has been improved by incorporating nickel and carbon nitride. Furthermore, electrocatalysis in terms of improved current density has been observed with increased surface area of the electrode. Moreover, the electrocatalyst materials have been characterized via techniques such as X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy and Raman spectroscopy. This work further involves the analysis of hydrogen evolution reaction performance at different pH levels.

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Activated Carbon from Spent Coffee: A Green Solution for Hydrogen Storage

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Abstract

Currently, due to escalating climate changes and energy crises, the need for alternative renewable energy sources has become crucial. In light of this, hydrogen has emerged as a green energy carrier. However, its shipment and storage pose major obstacles to its large-scale adoption. Although experts have managed to store hydrogen in various storage methods such as geological formations, pressure tanks, and liquid hydrogen, these storage systems suffer from limited capacity, low energy efficiency, high costs, and safety concerns. To address these challenges, reliable, safe, and efficient alternative technologies with high gravimetric capacity are crucial. Hydrogen storage in porous carbons is considered a promising technology due to rapid rate of hydrogen adsorption-desorption, natural abundance of raw materials, and good regeneration capacity, particularly in the context of automobile applications [1]. Despite encouraging findings regarding hydrogen storage capacities in carbon materials, no material is able to store 6.5 wt%, which was set by the U.S. Department of Energy (DOE) [2] at ambient temperatures and pressure. In this study, a readily available biomass waste derived from spent coffee grounds was used to produce high surface area activated carbon for hydrogen storage purposes. The coffee grounds were carbonized at three different temperature setpoints (350 °C, 400 °C, and 450 °C) and chemically activated with KOH in the presence of argon gas at a high temperature of 800 °C. The synthesized activated carbon samples were comparatively characterized using thermogravimetric analysis, scanning electron microscopy, and BET specific surface area analysis. The hydrogen uptake capacity of the activated carbons is determined using a gravimetric sorption analyzer. TGA analysis showed that all activated carbons exhibited higher thermal stability, maintaining more than 80% of their weight at 600 °C. The BET and SEM analysis also revealed a high surface area and well-developed porous structure suggesting their suitability for hydrogen storage applications. Activated carbons derived from spent coffee, possessing well-developed porosity and high specific surface area, exhibited promising hydrogen adsorption capacity. This study confirms that spent coffee activated carbon is a promising and sustainable hydrogen storage material, contributing to the decarbonization journey.

References

- [1] G. Sethia and A. Sayari, "Activated carbon with optimum pore size distribution for hydrogen storage," *Carbon N Y*, vol. 99, pp. 289–294, 2016, doi: 10.1016/j.carbon.2015.12.032.
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