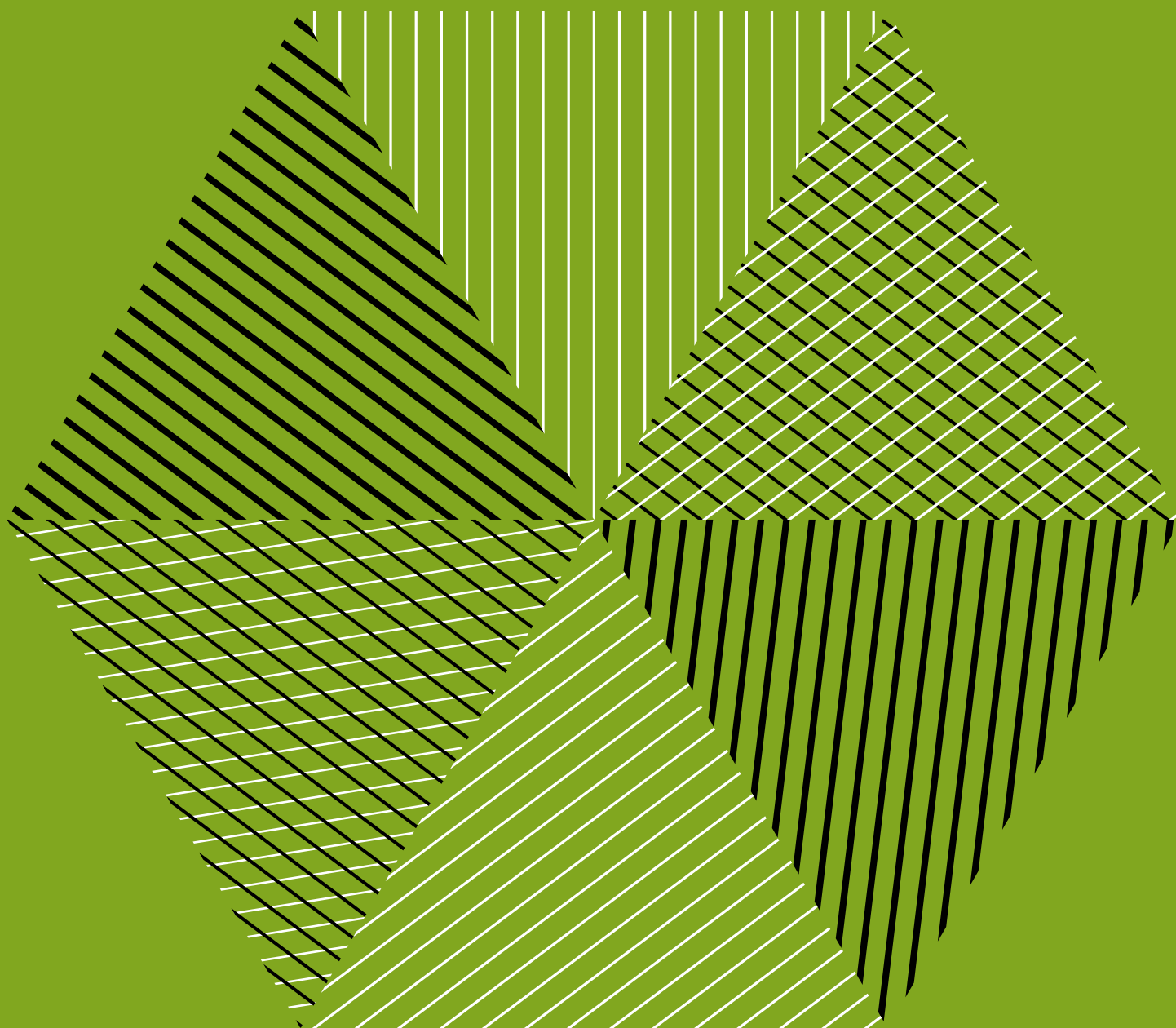


IOP Publishing

Energy 2025



A one-day event for early career researchers
on the future of energy research and the
green economy.

29 April 2025, IOP London

Energy 2025 Programme

Tuesday 29 April 2025

8:30 AM - 9:00 AM	Registration and Refreshments
9:00 AM - 9:15 AM	Welcoming Remarks
9:15 AM - 10:00 AM	Keynote 1 – Prof. Emma Kendrick (Batteries) Recycling and Reuse of lithium and sodium ion battery materials
10:00 AM - 10:45 AM	Keynote 2 – Prof. Petra Cameron (Photovoltaics) Why do we need new types of solar cell? The opportunities and challenges of next generation photovoltaics
10:45 AM - 11:15 AM	Morning Break
11:15 AM - 12:00 PM	Keynote 3 – Prof. Ifan Stephens (Power-to-X) Electrons at Work: Bridging Water Electrolysis, Nitrogen Reduction, and Battery Science
12:00 PM - 12:45 PM	Keynote 4 – Prof. Elizabeth A. Gibson (Circular Economy) A Circular Economy of Chemicals
12:45 PM - 1:45 PM	Networking lunch
1:45 PM - 2:30 PM	Keynote 5 – Dr. Jessica Higgins (Nuclear Energy) Conventional Nuclear Power Plants vs Small Modular Reactors: is bigger always better?
2:30 PM - 3:15 PM	Keynote 6 - Prof. Aron Walsh (AI for Energy) Can AI Discover Materials?
3:15 PM - 3:45 PM	Afternoon Break
3:45 PM - 4:45 PM	Careers Panel
4:45 PM - 6:15 PM	Posters, Networking, Drinks and Nibbles
6:15 PM - 6:30 PM	Closing Remarks and Poster Prizes

Keynote Speakers

'Why do we need new types of solar cell? The opportunities and challenges of next generation photovoltaics'

Prof Petra Cameron¹

¹*University of Bath, United Kingdom*

The UK government has a vision of generating clean, affordable and local power to the country by 2030 [1]. Photovoltaics will be an important component of the energy mix, and a strong UK based solar industry is important for our energy security. This talk will focus on the opportunities and challenges of next generation solar cells, including perovskite and dye sensitized solar cells. Researchers working on new types of solar have the exciting opportunity to design-in sustainable manufacturing and recycling processes from the very start, leading to new technologies that can slot easily into a circular economy.

[1] <https://www.gov.uk/government/publications/clean-power-2030-action-plan/clean-power-2030-action-plan-a-new-era-of-clean-electricity-main-report>

A Circular Economy of Chemicals

Prof Elizabeth Gibson¹

¹Newcastle University, United Kingdom

A sustainable resource flow of feedstocks must be integrated into an equitable and profitable chemicals value chain to support the transition to net-zero. Addressing this challenge requires interdisciplinary research that considers the complexity of supply chains and the diversity of stakeholders. By providing evidence for the viability of net-zero chemical technologies and a clear roadmap for implementation, future national chemical strategies can be de-risked and effectively deployed. We have been developing a roadmap for the Circular Economy of Olefins in the UK, based on the outcomes from the UKRI CircularChem centre. Barriers and opportunities will be discussed.

Our research shows that a fundamental shift in innovation culture is essential to achieving this transformation. Strengthening collaboration across the chemicals and chemicals-using sectors will drive investment and economic growth while reducing emissions and securing critical raw materials. With the global push towards net-zero becoming increasingly urgent, the UK chemical sector—contributing £48.7bn in annual turnover and supporting over 400,000 jobs—must adapt to maintain its competitive edge. The industry's reliance on fossil feedstocks presents a significant challenge, as it accounts for 10% of global energy consumption and could become the largest oil consumer by 2030. Despite chemicals representing only 5-7% of oil production, they contribute approximately 50% of oil revenue, underscoring the industry's economic significance. Creating a symbiotic relationship between net-zero initiatives and chemical manufacturing is key to success, ensuring that sustainability becomes an economically viable goal across the entire supply chain.

By integrating sustainable feedstocks, fostering digital innovation, and transforming industrial relationships, the transition to a resilient, net-zero chemical industry can be accelerated, positioning the sector as a leader in sustainable manufacturing. A case study on how high value materials can be extracted from waste will be presented to demonstrate how the circular economy can support both Net Zero greenhouse gas emissions and resource efficiency and resilience.

Conventional Nuclear Power Plants vs Small Modular Reactors: is bigger always better?

Jessica Higgins¹

¹Amentum, UK

The UK led the way in nuclear power production, with the first civil reactor being opened at Calder Hall, Cumbria in 1956. Spurred on by rising oil prices in the late 1960s, and the perception of nuclear as being 'strike-proof', a total of 37 reactors were built between 1956 and 1995. Nuclear power output peaked in the late 1990s with supply reaching 26% of the UK's total energy demand.

Of the 9 operational reactors remaining, 8 are UK designed Advanced Gas-Cooled Reactors (AGRs) and one is a Westinghouse Pressurised Water Reactor (PWR). Together, the UK's reactor fleet provides a steady supply of up to 15% of the total energy demand, equivalent to ~4.4 Giga Watt (GW) in 2024. However, all 9 reactors are due for decommissioning by 2035 unless plant life extensions can be agreed.

Only one new nuclear power plant is currently under construction in the UK at Hinkley Point C, Somerset. This European PWR EDF design houses two reactors with a power output of 1.6 GW each, 3.2 GW in total. This project has been beset with delays and the predicted total construction cost was reported by the BBC in 2024 to be over £46 billion on completion. Although this reactor will last for at least 60 years and supply ~10% of the UK's energy demand alone, the concern is that construction costs will be recuperated through higher consumer bills. Hinkley Point C is due to become operational in 2030.

Even with the construction of Hinkley Point C, the UK is predicted to have an energy deficit by 2040. Small Modular Reactors (SMRs) are being considered as an alternative to conventional large-scale reactors to bridge this shortfall. Their smaller size provides more flexibility in the supply chain to provide components. Plus some items can be partially build off-site and assembled in-situ (modular build). The International Atomic Energy Agency (IAEA) has reported that globally 45 different SMR designs are currently in development and 4 are under active construction. To date, two SMR designs have been approved under the initial Generic Design Assessment (GDA) regulatory phase for use in the UK. However, no firm orders have been placed and therefore operation dates are difficult to predict. Using a water cooled SMR as an illustrative example, power outputs are expected to be ~0.3 GW (with some going up to 0.5 GW) with construction cost estimated at anywhere between £500 million and £2 billion. This produces an estimated capital cost per Giga Watt of £6 billion, compared to over £14 billion per GW for Hinkley Point C. Cost savings for SMRs can be realised through economies of scale; the more units purchased, the cheaper the build process.

However, the requirement to build more units compared to a conventional reactor (i.e. 10 SMRs to 1 Hinkley Point C), potentially results in more waste generated over its lifetime and at decommissioning. At present, SMRs are in a relatively early stage of development. The dilemma for policy makers is whether to fund conventional reactors, based on well-known technology but at huge upfront capital costs, or diversify with SMRs and accept the unknown risks.

Recycling and Reuse of lithium and sodium ion battery materials

Prof Emma Kendrick¹

¹*University of Birmingham, United Kingdom*

This talk explores sustainability challenges in lithium-ion and sodium-ion battery technologies, with a focus on improving circularity and recovery efficiency across the battery lifecycle. Critical materials such as lithium, cobalt, and graphite pose supply chain risks, prompting interest in sodium-ion alternatives that use more abundant and lower-cost elements like sodium, iron, and hard carbon. However, the lower intrinsic value of sodium-ion materials, combined with contamination in traditional recycling routes, limits the quality and reuse potential of recovered products. Improving the purity and management of black mass, the mixed active material produced during mechanical sorting, is essential. Direct recycling offers a viable route if black mass purity can be sufficiently controlled, allowing for the regeneration of cathode materials without complete breakdown. This work considers battery design, manufacturing, and end-of-life processing together, highlighting opportunities to improve material circularity through design-for-disassembly and targeted recycling strategies for both lithium- and sodium-based chemistries.

Electrons at Work: Bridging Water Electrolysis, Nitrogen Reduction, and Battery Science

Professor Ifan Stephens¹

¹*Imperial College London, United Kingdom*

Electrochemistry is central to our transition to a net zero society. While fuel cells and batteries are poised to decarbonise transport, electrolyzers offer a route to sustainably produce vital chemicals such as hydrogen and ammonia. Intriguingly, some of the same reactions we aim to accelerate—like hydrogen evolution in water splitting—are exactly those we seek to suppress in other technologies, such as lithium-ion batteries and nitrogen reduction systems.

In this talk, I will show how our group navigates this complex landscape by translating techniques and insights across these interconnected areas. I'll present our recent mechanistic studies on:

- (i) oxygen evolution on iridium-based oxides for water electrolysis,
- (ii) nitrogen reduction to ammonia in organic electrolytes, and
- (iii) parasitic gas evolution in lithium-ion batteries.

We combine electrochemical measurements with a broad suite of complementary techniques—including electrochemical mass spectrometry, operando optical spectroscopy, secondary ion mass spectrometry, cryo-electron microscopy, x-ray photoelectron spectroscopy, and density functional theory—to develop a holistic view of these key electrochemical processes.

Can AI Discover Materials?

Aron Walsh¹

¹*Imperial College London, United Kingdom*

Integrating artificial intelligence (AI) into materials research prompts a re-evaluation of traditional discovery paradigms. Advances in computational hardware, from high-performance supercomputers to emerging quantum processors, are now complemented by sophisticated software that deciphers complex structure–property relationships [1]. I will discuss whether modern AI techniques—including deep learning, generative models, and reinforcement learning—can transcend conventional workflows to identify truly novel materials [2]. By analysing recent case studies in clean energy and other sectors, the talk will assess the reproducibility, interpretability, and practical impact of AI-driven discovery platforms. Critical challenges such as data quality, standardisation, and model validation [3] will also be discussed, questioning whether the current infrastructure is sufficient to support scientific breakthroughs.

[1] “Machine learning for molecular and materials science” *Nature* 559, 547 (2018)

[2] “Has generative artificial intelligence solved inverse materials design?” *Matter* 7, 2355 (2024)

[3] “Open computational materials science” *Nature Materials* 23, 16 (2024)

Poster Presentations

Gel electrolytes based on cellulose acetate and a high lithium concentration phosphonium ionic liquid for high performing lithium-ion batteries

Dr Onajite Theresa Abafe Diejomaoh¹, Stephen J. Eichhorn¹

¹*University Of Bristol, Bristol Composite Institute, United Kingdom*

Conventional lithium-ion batteries contain organic solvents as electrolytes, which are highly flammable and prone to leakage, requiring replacement with less volatile and mechanically stable electrolytes. In addition, due to the urgent need to transition to more sustainable electrolytes, gel polymer electrolytes based on cellulose have received attention for their abundance, sustainability, and mechanical flexibility. However, current gel polymer electrolytes based on cellulose still require improvement to attain higher conductivity and interfacial compatibility to enable their use as electrolytes. Ionic liquids, which have unique properties, including high conductivity, high thermal stability, low flammability and low vapour pressure, are suitable alternatives to organic electrolytes in lithium ion batteries. In this work, a novel gel polymer electrolyte based on cellulose acetate and a high lithium concentration phosphonium ionic liquid, 3-aminopropyl-tributylphosphonium bis(trifluoromethylsulfonyl) imide ([aP4443][NTf2]) were prepared by solution casting method. The composition-dependent behaviour of the components in the GPE is investigated by differential scanning calorimetry (DSC), electrochemical impedance spectroscopy (EIS), Fourier transform infrared spectroscopy (FTIR), and tensile testing. The effects of adding cellulose nano-fibres to the polymer electrolyte were also analysed. Introducing high lithium-concentration ionic liquids into the cellulose acetate is expected to effectively decrease the glass transition temperature (T_g) of the resulting GPE, leading to improved ion dynamics and higher ionic conductivity. The cellulose nano-fibres will effectively increase the mechanical stability of the GPEs to finally yield a highly conductive free-standing GPE membrane suitable for lithium-ion batteries.

Exsolution of Ultrasmall Pt Nanoparticles on High-Surface Area Mesoporous Assemblies of $\text{La}_{0.985}\text{Ba}_{0.015}\text{Al}_{0.99}\text{Pt}_{0.0103}/\text{Al}_2\text{O}_3$ Towards Superior Selective Catalytic Oxidation of Ammonia

Mina Ardani¹, John T.S. Irvine¹

¹*University of St Andrews, United Kingdom*

Ammonia (NH_3) pollution deriving from the selective catalytic reduction (SCR) systems is a major environmental concern due to the harmful effects of the NO_x species produced during ammonia oxidation [1,2]. To minimize the NH_3 pollution materials that take part in the selective catalytic oxidation (SCO) of ammonia are being investigated and utilized. Platinum (Pt)-based catalysts are among the most promising candidates due to their high oxidation capabilities but their high manufacturing costs limit their industrial applicability. Exsolution of metallic nanoparticles from perovskite oxides has shown remarkable catalytic potential providing high activity accompanied by low cost and excellent chemical stability [3,4]. In this study, we present a novel synthetic method of devising nanoporous catalysts of $\text{La}_{0.985}\text{Ba}_{0.015}\text{Al}_{0.99}\text{Pt}_{0.0103}/\text{Al}_2\text{O}_3$ exhibit high specific surface area and nanoscale composition. Combined with the exsolution of ultrasmall Pt nanoparticles as catalytic active sites, the SCO- NH_3 is enhanced, utilizing only trace amounts of Pt. The nanoporous structure of the catalysts facilitates a better diffusion pathway of NH_3 through the mesoporous, while the presence of Pt nanoparticles further increases the catalytic activity by providing a plethora of catalytic active sites. The findings highlight the importance of exsolution as possible SCO- NH_3 catalysts that exhibit high catalytic activity, chemical stability, and affordability.

- [1] L. Chmielarz et al (2015), RSC Adv. 5, 43408-43431.
- [2] T. Lan et al (2020) Catal. Sci. Technol. 10, 5792-5810.
- [3] S. Ozkan et al (2024) Adv. Energy. Mater. 14, 230325.
- [4] D. Neagu et al (2023) J. Phys. Energy 5, 031501.

Symmetric double-layer capacitor with natural rubber and sodium salt-based solid polymer electrolyte and reduced graphene oxide electrodes

Dr Nilanthy Balakrishnan¹, Kumudu. S Perera², Kamal. P Vidanapathirana², Lewis. J Adams¹, Chris. S Hawes¹

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Solid polymer electrolytes (SPEs) are the key to improving electrochemical devices' energy density and safety. In recent years, natural polymers have received tremendous attention due to the latest advances in green technology for a sustainable future. Herein, SPEs based on 49% methyl grafted natural rubber (MG49-NR) and sodium trifluoromethanesulfonate (Na(CF₃SO₃) – NaTF) salt were prepared and characterized to optimize their performance [1]. The composition MG49-NR: NaTF = 1:0.5 (by weight) shows the highest room temperature conductivity of 7.52×10^{-4} S/cm. This optimized electrolyte is purely an ionic conductor with an activation energy of 0.29 eV. The optimized electrolyte was used to fabricate double-layer capacitors by sandwiching it between two identical reduced graphene oxide (rGO) electrodes. The fabricated double-layer capacitors show a maximum single electrode specific capacitance (C_{sc}) of 42.5 F/g from the cyclic voltammetry (CV) test. Moreover, the charge storage mechanism utterly takes place via non-faradaic reactions which is evidenced by cyclic voltammograms. Furthermore, the electrochemical impedance spectroscopy (EIS) test shows the capacitive features are dominant at low frequencies. Performance of the double-layer capacitor during 10,000 charge and discharge cycles at a constant current density of 0.05 A/g shows a fast drop of single electrode specific discharge capacitance (C_{sd}) at the beginning, but it started to saturate after the 5,000th cycle proving the good stability of the capacitor. These findings are relevant to expanding the functionalities of double-layer capacitors having natural rubber-based SPEs in green technologies.

Reference

[1] K.S. Perera et al., Journal of Energy Storage, 97, 112683 (2024).

Corrosion Behaviour of the Zinc Anode in Aqueous Zinc-ion Batteries (Poster Presentation)

Prof Habibat Chahul^{2,1}, James Simon¹, Jessica O'Flaherty¹, Svetlana Menkin¹, Clare P. Grey¹

¹Yusuf Hamied Department of Chemistry, University of Cambridge, United Kingdom, ²Joseph Sarwuan Tarka University Makurdi, Nigeria

Large-scale battery technologies are central to establishing a grid-scale energy storage system and global decarbonization. Rechargeable aqueous zinc-ion batteries (AZIBs) are of significant interest due to their low cost, excellent operational safety, and more, environmental friendliness. However, challenges arise from the mildly acidic pH of the zinc salt electrolytes and the competing hydrogen evolution process during zinc electrodeposition. These factors lead to corrosion processes induced by hydroxide ions, resulting in the formation of dendrites and irreversible degradation of the metallic zinc anode, which pose considerable barriers to the practical applications of metallic zinc anodes and further advancements of zinc-ion batteries. A thorough investigation into the underlying causes of this issue is crucial for the large-scale deployment of AZIBs. This study reports on the corrosion thermodynamics and kinetics of zinc electrodes in aqueous electrolyte systems of zinc salts, employing voltammetry, linear polarization resistance (LPR), pH measurements, electrochemical impedance spectroscopy, and optical microscopy. Attempts have been made to enhance the stability of the zinc anode with a green additive. Our findings provide valuable insights into tackling the instability of the zinc anode in AZIBs, therefore paving the way for their practical application.

Up-scaling photoelectrochemical reactors – lab-scale optimisation to outdoor field testing

George Creasey¹, Arend Moelich², John W. Rodriguez Acosta¹, Thomas Shalvey³, Alicia Garcia-Osorio³, Jinjie Zhu¹, Sid Halder¹, Jon Major³, Alex Cowan³, Craig McGregor², Andreas Kafizas¹, Anna Hankin¹

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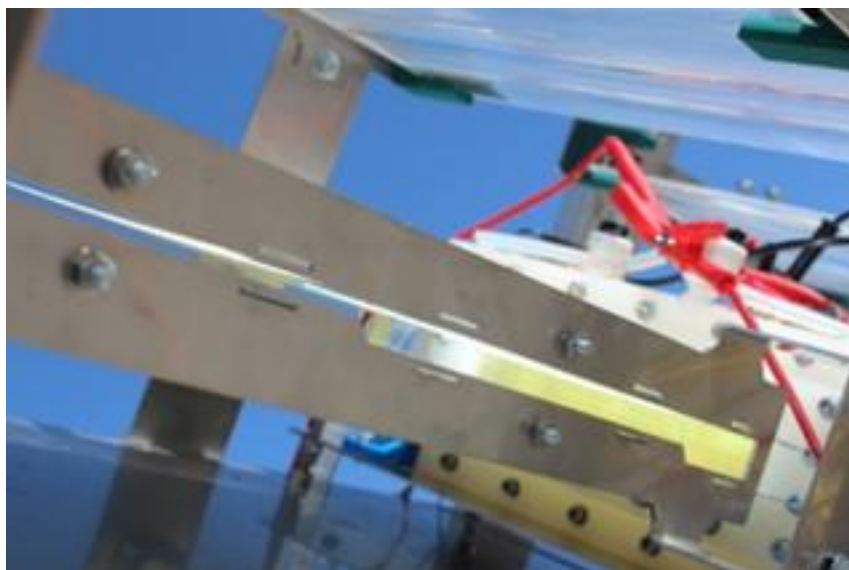
Research in photoelectrochemical (PEC) hydrogen production remains primarily focused on materials development, with few studies addressing devices. Taking PEC hydrogen production from the lab towards commercialisation requires a whole systems approach in which the device and materials design are addressed in parallel. Several constraints on photoelectrode materials and photoelectrochemical devices must be considered simultaneously. These include: (i) electrode scalability; (ii) modes of illumination; (iii) current distribution on the electrodes; (iv) heat and mass transport [1]. Alongside these considerations, photoelectrode materials must harness light over a wide range of wavelengths, catalyse water oxidation/reduction, and be chemically, (photo)electrochemically and mechanically robust.

Our up-scaled photoelectrochemical reactor (Fig. 1) was tested outdoors with natural sunlight at the Stellenbosch University solar rooftop laboratory testing facility (33.93° S, 18.86° E). The 60 cm² reactor was mounted on a two-axis tracking platform, with light directed laterally onto both the photoanode and photo(cathode) sides, either with reflected or concentrated (up to four times) irradiance.

The reactor was operated in two modes:

- (i) Photoelectrochemical (PEC), with an FTO | WO₃ | BiVO₄ | NiFeOOH photoanode and a FTO | Au | Sb₂Se₃ | CdS | TiO₂ | Pt photocathode [2].
- (ii) PV-assisted photoelectrochemical (PV-PEC), with an FTO | WO₃ | BiVO₄ | NiFeOOH photoanode, Ni cathode and externally mounted c-Si PVs.

I shall discuss experimental results from reactor testing, including associated difficulties of taking experiments from a controlled lab facility to an outdoor testing environment, and the performance of the reactor, operated in different modes and configurations.



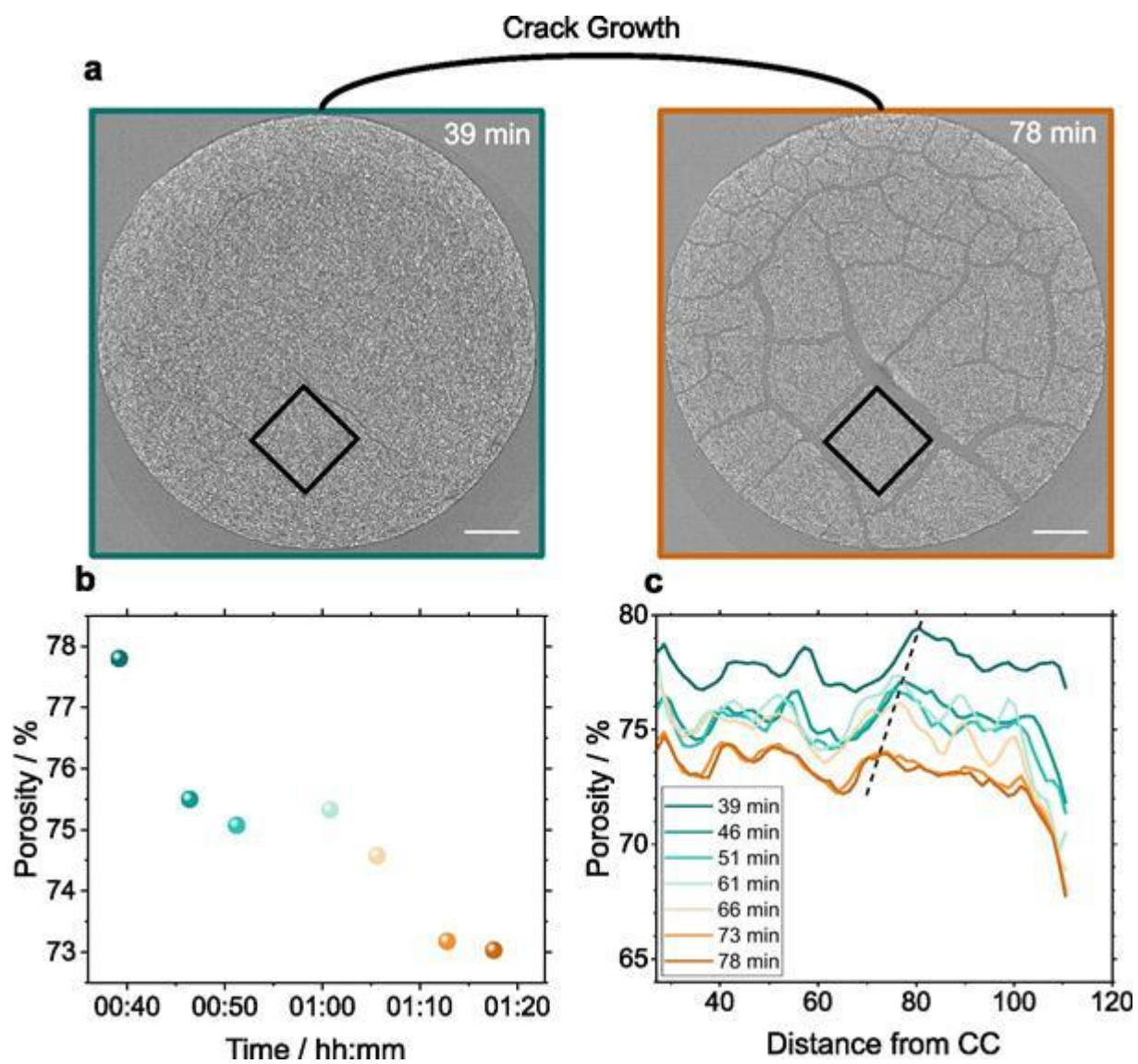
Predicting Crack Formation in Drying Slurry Cast Electrodes with In Situ X-ray CT

Will Dawson², Andrew Morrison¹, James Robinson², Paul Shearing³

¹Electrochemical Innovation Lab, UCL, United Kingdom, ²Advanced Propulsion Lab, UCL, United Kingdom, ³Zero Institute, University of Oxford, United Kingdom

Mud cracking is the process of electrode-level fracture which occurs during the electrode drying process. Cracking is a major limitation to the production of thick Li-ion electrodes, particularly as the industry moves towards aqueous processed cathodes and smaller active particles.^{1,2} The proposed mechanism for crack suggests that solvent drying proceeds as a liquid evaporating from the meniscus surface in a porous network, thus creating capillary pressure which results in the opening of cracks in the electrode. The same principles apply to other slurry-processed energy materials including solar cells and other battery chemistries.^{3,4} Existing studies on electrode drying and microstructural formation have visualised the structure in 2D, and have shown that binder, key in limiting cracking, forms largely between closely-packed particles.⁵ Crack structure is naturally 3 dimensional, and this informs the nature of crack formation and their influence of electrode performance.⁶ In this work the electrode drying process was imaged in situ and in 3 dimensions for the first time. The evolution of electrode microstructure is related to crack formation, and image analysis tools are applied to predict crack location based on local microstructures.

- 1 Du et al., J. Power Sources, 2017, 354, 200–206.
- 2 Bresser et al., Energy Environ. Sci., 2018, 11, 3096–3127.
- 3 Weerasinghe et al., Nat. Commun., 2024, 15, 1656.
- 4 Zhao et al., J. Power Sources, 2019, 413, 259–283.
- 5 Jaiser et al., J. Power Sources, 2017, 345, 97–107.
- 6 Dawson et al., Batter. Supercaps, 7, 12.



Reappraisal of paths to decarbonising GB electricity generation in 2030

David J Dunstan¹, Alan J Drew¹, Alfonso San Miguel²

¹Queen Mary University of London, United Kingdom, ²University of Lyons, France

The UK Government plans to bring forward the decarbonisation of British electricity generation from 2035 to 2030, and the UK NESO has provided details of how this may be achieved by adaption of the previous strategy for 2035. It is timely to reconsider from first principles the 2035 plans as adapted for 2030. Analysing the 2023 electricity generation data, we find that the problems caused by the intermittency of wind and solar generation have been grossly underestimated. Both surpluses and deficits of renewable generation are much larger and more frequent than assumed. We model two paths to 2030 with simplifications designed to reveal the underlying principles more clearly. Key findings are:- expansion of electrification before 2030 aggravates the worst problem of intermittency (deficits) without any proven savings yet in carbon emissions; abatement of the CO₂ emissions from fossil gas use by carbon capture and sequestration – if feasible – should be introduced and expanded as fast as possible both to handle the deficits and as an immediate and independent action to rapidly reduce CO₂ emissions; and sheddable loads such as electrolysis of hydrogen and synthesis of hydrocarbons need to be introduced to exploit the surpluses of renewable generation and store them.

Lithium-ion high power cell: Lithiumwerks 26650 Battery Parameterization

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¹*University of Birmingham, United Kingdom*

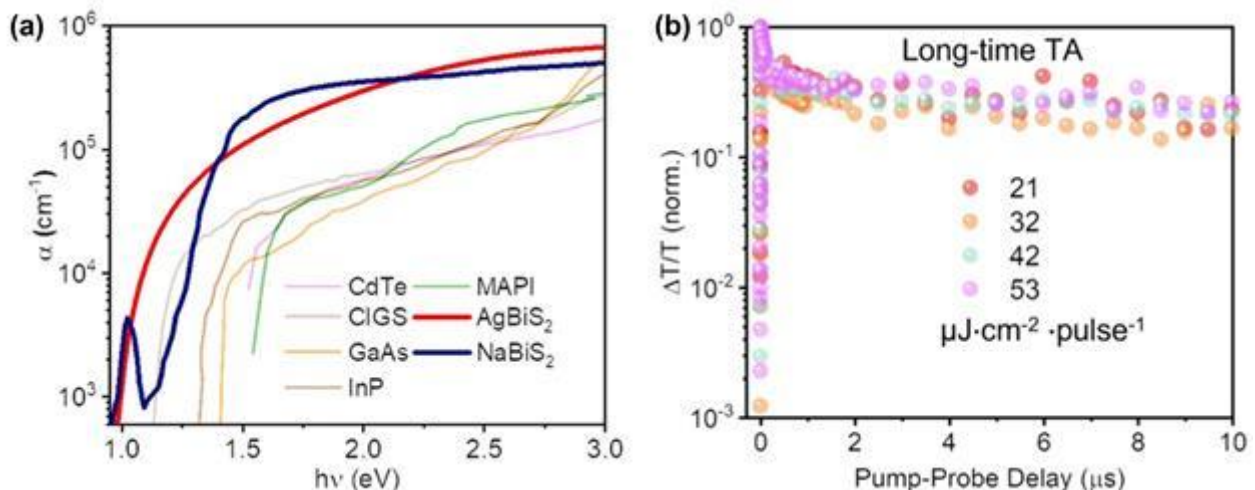
Lithium-ion batteries play a critical role in high-power applications such as in electric vehicles, energy storage and aerospace due to their thermal stability and long cycle life. Lithiumwerks 26650 is a high power LiFePO₄ cell with Nanophosphate battery technology. To optimise performance, enhance lifespan and ensure safety of the battery, accurate parameterization is required. Finding suitable parameters to simulate a battery is one of the main challenges in battery modelling. This work focuses on the experimental parameterization of Lithiumwerks 26650 cell for a more accurate model prediction by extracting key physical, chemical and electrochemical properties required for precise simulation. Physical parameters include the cell and cell components' dimensions, weight, porosity etc. Chemical parameters encompass the active material composition and crystal structure. Electrical parameters such as cell capacity and efficiency, open-circuit voltage (OCV), internal resistance and diffusion coefficients are obtained. These parameters will then be integrated into P2D models to investigate the battery performance through state-of-charge and state-of-health estimations. Accurate parameterization is crucial for applications demanding high efficiency and safety. By refining battery models with precise data, this research helps bridge the gap between theoretical design and real-world operation, ultimately supporting the efficient deployment of high-power and high-energy lithium-ion technologies.

A study on the optoelectronic properties of an emerging perovskite-inspired material - NaBiS₂

Yi-Teng Huang¹, Seán Kavanagh², Marcello Righetto³, Akshay Rao⁴, Laura Herz³, David Scanlon⁵, Aron Walsh⁶, Robert Hoyer¹

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The efficiency of perovskite solar cells has increased rapidly over the past decade, recently reaching levels comparable to crystalline silicon solar cells. Beyond their excellent optoelectronic properties, this progress is largely due to perovskites' unusual defect tolerance, which allows high-performance devices to be fabricated through simple solution-processing methods. However, the presence of toxic lead and poor air stability in perovskites significantly hinder their commercial viability. These challenges drive the search for lead-free alternatives, known as perovskite-inspired materials (PIMs), that might replicate perovskites' defect tolerance. In this work, we present a comprehensive study on the optoelectronic properties of an emerging air-stable PIM, NaBiS₂. We demonstrate that NaBiS₂ exhibits absorption coefficients higher than most thin-film photo-absorbers, with a sharp absorption onset and an exceptionally long carrier relaxation time exceeding 10 micro-seconds (see the attached Figure 1). Moreover, the carrier dynamics of NaBiS₂ appears unaffected by the introduced defects, which to some extent, also suggests the defect tolerance of this material. Interestingly, our density functional theory calculations reveal that these properties may stem from non-bonding sulfur p orbitals and intrinsic cation disorder, which also lead to strong carrier localization. Through the ligand-exchange treatment on NaBiS₂, we prove that despite the improved carrier transport in different length scales, carrier localization remains in its photoconductivity transients. As a result, the performance of NaBiS₂ devices is still limited so far. This work hence highlights the critical influence of the electronic band structure on both the absorption features and carrier dynamics of PIMs.



Lithium Ionic Conductors from the Li₃PS₄-Li₄SiS₄

Binary Thio-LISICON System

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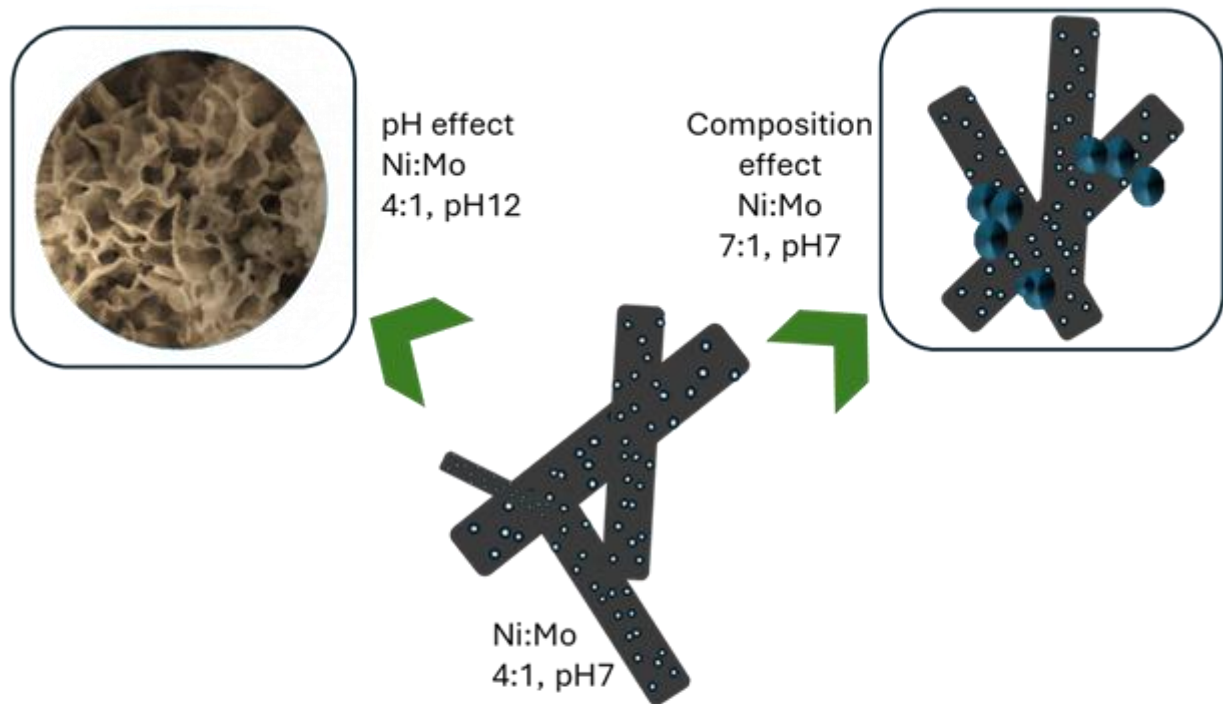
The rising demand for electrochemical energy storage has driven advancements in battery technology. While Li-ion batteries (LIBs) remain dominant for electric vehicles, their flammable liquid electrolytes pose safety risks. All-solid-state batteries (ASSBs) offer a promising alternative, with sulfide solid electrolytes (SEs) being particularly attractive due to their high ionic conductivity and mechanical properties. Among these, Thio-LISICON materials (Li_xM_xS₄, M=P, Si, Sn, Ge) are of interest. This study investigates the Li₃PS₄-Li₄SiS₄ system, focusing on silicon (Si) for its abundance, lower toxicity, and cost-effectiveness compared to germanium (Ge). Various compositions (x=0.4, 0.5, 0.6) were synthesized using ball-milling and melt-quenching. While melt-quenching requires impractically high temperatures (>1050 °C), ball-milling achieved a conductivity of 10⁻⁵ S/cm at room temperature, which improved to 10⁻³ S/cm after heat treatment at 550 °C. The x=0.6 composition demonstrated superior conductivity due to its crystalline structure's similarity to LGPS rather than the Thio-LISICON I group. With further research, this system could yield safer, more cost-effective, and stable electrolytes, accelerating the transition to green, emission-free energy solutions

Optimization of Powdered NiMo Electrocatalysts for Hydrogen Evolution Reaction: Influence of pH and Ni Composition

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¹*School of Chemistry and Chemical Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, United Kingdom*, ²*School of mechanical engineering sciences, Faculty of Engineering and Physical Sciences, University of Surrey, United Kingdom*

To achieve net-zero carbon goals, transitioning to hydrogen technologies is essential, with AEM water electrolysis offering highly pure and renewable hydrogen. Developing cost-effective, efficient, and stable powdered electrocatalysts for HER is crucial for commercial hydrogen production. A NiMo alloy has been recognized as a benchmark catalyst for HER, with the best HER activity reported for NiMo alloy growing directly on Ni foam[1–3], which is not easy to be assembled in commercial electrolyzers. Herein, we aim to develop and optimize powdered NiMo alloy using hydrothermal reaction as HER electrocatalysts. The optimal pH environment and Ni composition in the precursor were investigated to enhance the performance of the NiMo alloy compared to platinum. X-ray diffraction (XRD) and X-ray spectroscopy (XPS) analysis confirmed that NiMo alloy particles were successfully synthesized. Microstructural analysis using scanning electron microscope (SEM) revealed a transition from nanorod to floral morphology as the pH shifted from slightly acidic to highly alkaline, though this change did not significantly improve catalytic activity. HER activities of the synthesized catalysts were tested using a rotating disk electrode (RDE) in alkaline media of 1 M KOH solution. pH 7 was identified as the most favourable environment for precursor reactions, leading to the formation of an active catalytic phase. Furthermore, the Ni to Mo mole ratio was varied (4:1, 5:1, 6:1, 7:1, & 8:1) to optimize HER performance in a neutral pH environment. These contributions will help to further explore the possibility of using the non-precious electrocatalyst at commercial scale for hydrogen production.



1. Fang, M. *et al.* Hierarchical NiMo-based 3D electrocatalysts for highly-efficient hydrogen evolution in alkaline conditions. *Nano Energy* **27**, 247–254 (2016).
2. Cao, J. *et al.* Hierarchical NiMo alloy microtubes on nickel foam as an efficient electrocatalyst for hydrogen evolution reaction. *Int J Hydrogen Energy* **44**, 24712–24718 (2019).
3. Zhang, J. *et al.* Efficient hydrogen production on MoNi₄ electrocatalysts with fast water dissociation kinetics. *Nat Commun* **8**, (2017).

Investigating the impact of mechanical strain on the optoelectronic properties of metal halide perovskites in four dimensions

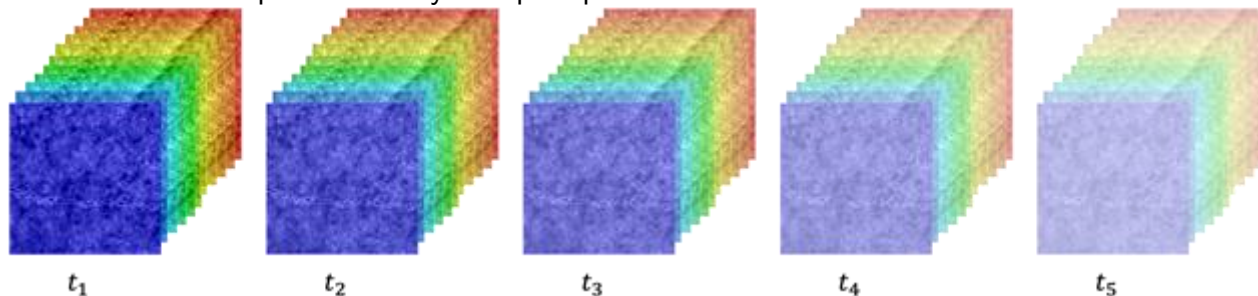
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Perovskites are a promising class of materials for next generation solar cells. Whilst metal halide perovskite solar cells have demonstrated high efficiencies for lab grown devices, the instability of these devices is a key obstacle which must be overcome to start widespread commercial implementation. Strain engineering is proposed to be a promising approach to improve this stability, but nominally similar perovskites under near-identical strain conditions can exhibit very different charge carrier dynamics making it hard to successfully implement. This poster will present results showing the impact of mechanical strain on the charge carrier recombination dynamics of CsPbBr₃ microcrystals. We developed a time-resolved hyperspectral microscope which can be employed to observe the optoelectronic properties of perovskites with sub-nanosecond resolution across a wide spectral range. Dynamic range of eight orders of magnitude has been achieved with this time-resolved system, meaning that decays can be detected hundreds of microseconds after initial excitation.

We applied mechanical tensile stress in situ to CsPbBr₃ microcrystals and used the developed microscopy system to collect spectrally resolved photoluminescence spatial maps and time-resolved photoluminescence spatial maps. It is shown that application of tensile strain changes the intensity of the emitted photoluminescence without evidently changing the spectral shape of this emission. Photoluminescence decays are also presented showing how the application of tensile strain impacts defect concentrations and recombination within the material.

It is also shown how the developed system can be used to track the z-diffusion of charge carriers within the perovskite crystals post photoexcitation.



Semiconducting Materials from Analogy and Chemical Theory

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As the number of chemical components increases, there is a combinatorial explosion in the number of possible compounds. Mapping from compositions to structures has been a longstanding bottleneck in large-scale materials informatics workflows. Our current approach is to integrate chemical rules, generative AI, and machine learning forcefields into a powerful workflow for materials discovery.

The original SMACT code used a liberal set of oxidation states to explore configurational spaces. While this approach enabled broad exploration, it often included unstable or implausible combinations. We now aim to implement stricter oxidation state filters based on the occurrence of oxidation states and their combination in the inorganic crystal structure database (ICSD). By narrowing the range of oxidation states, this study will provide a more focused and reliable prediction of stable materials, ensuring that the generated candidates are experimentally viable and energetically favourable.

The first stage of screening involves the application of machine learning forcefields for ternary inorganic compounds, with the most competitive candidates then subject to density functional theory calculations. The second aspect is targeting specific structure types, with an initial focus on “missing” spinels, i.e. compositions that are plausible in the spinel structure but have not yet been observed. Our goal is to predict the synthesizability parameters to rank the possibility of each spinel being synthesised. The results of this study provide valuable insights into the spinel compositional space and serve as a fundamental building block for developing a workflow to investigate novel materials for green energy and advanced technology applications.

Spectroscopic insights into the electrochemical origins of quasi-Fermi level splitting in Fe₂O₃ photoanodes

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Photovoltage is the additional driving force generated in semiconductors under illumination. In solar cells, this is measured as the open circuit voltage across the device, which matches the quasi-Fermi level splitting (QFLS). In photoanodes for photoelectrochemical (PEC) water splitting, understanding the QFLS is complicated by three key factors: (1) the single electrical contact in photoanodes makes direct operando measurements of QFLS difficult; (2) water oxidation is a slow redox process; and (3) these systems are often operated under applied bias, where the band alignment is different to open circuit conditions.

In this work, we use pump-probe spectroscopy to measure the QFLS of Fe₂O₃ by directly probing hole populations. We aim to investigate QFLS as a function of light intensity and to understand its relationship to the photovoltage obtained from current-voltage curves. Our results provide direct experimental evidence that the QFLS in photoanodes under applied bias is driven by electrochemical populations, and that this differs from the electrostatic change in band bending observed under open circuit conditions. We also observe pinning of the hole quasi-Fermi level ($E_{F,p}$) to states close to the valence band edge (VBE) which are not active for oxygen evolution. Pinning of the $E_{F,p}$ to these states occurs under conditions of first order water oxidation behaviour, while under conditions of third order behaviour, the $E_{F,p}$ moves closer to the VBE with increasing light intensity.

Investigation of Ion Solvation on Sodium-ion Diffusivity in Hard Carbon

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Sodium-ion battery parameterization for a physics-based model involves physical, chemical, and electrochemical characterization of battery components and their behaviour in relation to different environmental impacts on energy storage and longevity. The ion diffusion action to the electrode reaction determines overall battery performance and health. In this study, we intrinsically understand that Na-ion solvation significantly influences the diffusion of Na-ions within the complex carbon anode. We employed intermittent current interruption (ICI) measurements to investigate Na-ion diffusion in hard carbon under two electrolyte solvent environments: carbonate-based and ether-based. Notably, the carbonate-based electrolyte exhibited lower diffusivity than the ether-based electrolyte, a difference attributed to Na-ion solvation, electrolyte viscosity, and ionic conductivity. Additionally, electrochemical impedance spectroscopy revealed that both internal conductivity and intercalation in the ether-based electrolyte were faster and more efficient than those in the carbonate-based electrolyte. These findings underscore the necessity of establishing precise parameters for Na-ion batteries to inform the design and production of future Na-ion battery energy storage technologies.

COMPUTATIONAL INVESTIGATION OF CALENDERING EFFECTS ON ELECTRODE STRUCTURE AND PERFORMANCE USING DISCRETE ELEMENT METHOD

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¹University Of Surrey, United Kingdom

Calendering is a crucial method in the fabrication of lithium-ion battery electrodes, as it significantly improves the structural, mechanical, and electrical properties. This study utilized two distinct approaches to simulate the calendering process using the discrete element method (DEM), to evaluate the structural analysis of NMC-622 electrodes: A Uniaxial (flat plate) compaction and Roller compaction. Uniaxial compaction provides structural information at the contact point between the roller and electrode; however, roller compaction captures a more realistic structural evolution and deformation as it introduces both normal and shear forces. A comparative study was performed to understand the calendering effect on porosity, stress distribution, tortuosity, and electronic conductivity. Furthermore, we assess the contact area of NMC particles with a current collector under different compression levels. The findings indicate that increasing compression enhances particle connectivity, and charge transport efficiency. For the first time, this study simulates an adhesion test using DEM to observe the adhesion strength of the electrode with the current collector. These observations contribute to optimizing the calendering parameters to attain higher electrode density, structural stability, and excellent electrochemical performance.

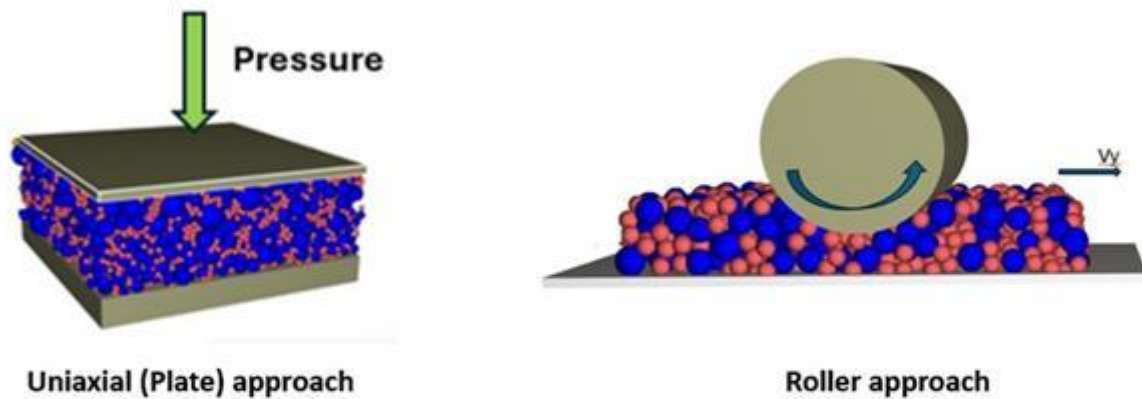


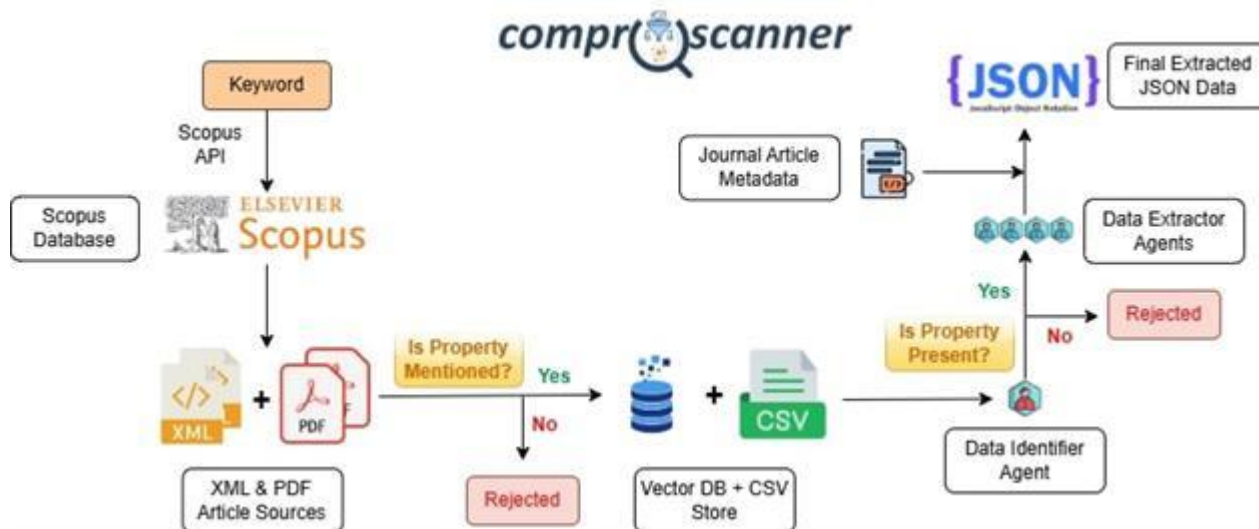
Figure 1. Two distinct calendering approaches

ComProScanner: A multi-agent based agile framework for high quality composition-property structured data extraction from scientific literature

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In this presentation we will describe ComProScanner, a multi-agent based cost-efficient scalable automated workflow for extracting, validating, categorising, and visualising machine-readable structured chemical compositions and properties, combined with synthesis information from journal articles to create extensive databases. Our system combines large language model (LLM) agents with powerful tools including Retrieval-Augmented Generation (RAG) and custom scripts for extracting chemical compositions and properties when only property values are available in articles. The workflow supports Elsevier, Springer, IOPScience, and Wiley articles via publishers' TDM (Text and Data Mining) APIs or PDFs from local folders. ComProScanner enhances text-mining accuracy by providing flexible contextual parameters to agents while maintaining cost-effectiveness through preliminary article filtering via keyword matching. The system supports multiple configurable LLMs for both extraction agents and RAG implementations. Finally, we will describe our evaluation of the system, where we processed 9,728 Elsevier articles on piezoelectric materials, with over 8,000 filtered using relaxed keyword matching for the property d33. Structured compositions and properties were subsequently extracted with high accuracy from 167 articles, demonstrating the workflow's effectiveness for creating specialised materials property databases. The framework exhibits the promise of scalability, enabling extraction of any user-specified material property to build extensive databases for data-driven materials design.



Powering the Future: Metal-Organic Nanosheets for Integrated Solar Energy Capture and Storage

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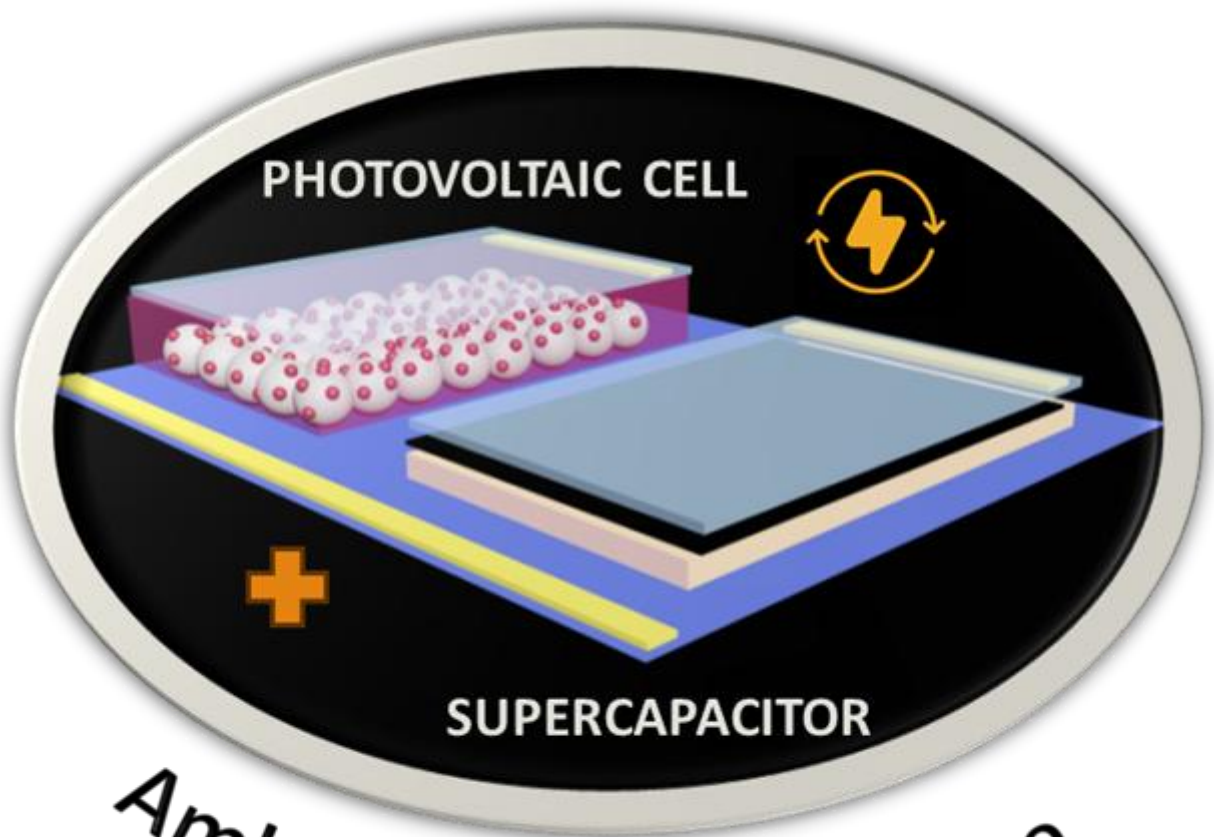
Integrating energy storage directly onto solar cells is a game-changer for renewable energy. Conventional solar cells generate electricity only when exposed to sunlight, requiring separate storage systems that add complexity and cost. This research introduces metal-organic nanosheets (MONs) as a novel solution, seamlessly merging energy generation and storage in a single device.

MONs are two-dimensional materials composed of metal ions and organic linkers, forming highly tunable molecular structures. By optimizing their conductivity and electrochemical properties, MONs serve as efficient interface materials in photovoltaic devices. A modulator-assisted synthesis method enables the self-assembly of MONs into continuous films with 1D ion-conducting channels, ensuring seamless charge transport and storage.

When integrated as capacitive electrodes with hybrid solar cells, MONs enable energy-storable solar devices with competitive power conversion efficiencies. Characterization using Grazing-Incidence Wide Angle X-ray Scattering confirms their guided orientation for optimal charge transport. Electrochemical impedance spectroscopy and galvanostatic charge-discharge measurements demonstrate excellent cycling stability, durability, and long-term charge retention.

By addressing limitations in traditional solar cells and supercapacitors, MON-integrated solar devices eliminate the need for separate storage systems, making energy solutions more compact and efficient. This breakthrough offers a scalable approach to sustainable energy storage, paving the way for next-generation solar technologies that are self-sustaining, cost-effective, and environmentally friendly.

MONs represent a paradigm shift in renewable energy, unlocking the potential for all-in-one solar power and storage solutions that can revolutionize the future of clean energy technology.



Ambient energy storage

Synergistic effect of trimetallic SnBiCu nanoparticles decorated on graphene oxide as high efficient electrocatalyst for fuel cell application

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Metal based nanocomposite's have significant applications in energy storage devices, but graphene oxide based nanocomposite's are more well known for their ability to improve electrochemical characteristics. The synthesized composite was thoroughly examined utilizing a number of techniques, including fourier transform infrared spectroscopy, scanning electron microscopy & energy dispersive X-ray spectroscopy, UV-visible spectroscopy and thermogravimetric analysis and differential scanning calorimetry. Cyclic voltammetry and electrochemical impedance spectroscopy were used to examine the electro-oxidation behaviors of methanol (MOR) on the SnBiCu@GO-modified electrode in an alkaline media at different concentrations of KOH, NaOH and KNO₃. When compared with different electrolytes, the SnBiCu@GO nanocomposite with KNO₃ electrolyte exhibited improved electrocatalytic efficiency and durability towards the oxidation of methanol. The value of "n" notably with n=6 for methanol determined the electrocatalytic behavior of the nanocomposite. Based on the outcomes of cyclic voltammogram data, the diffusion coefficients was measured within the range of 10⁻¹³ to 10⁻¹⁰ cm²/s and the rate constant falls between 10⁻⁷ to 10⁻⁵ cm/s. Charge transfer resistance (R_{ct}) falls within the range of 13-78Ω and solution resistance (R_s) falls within the range of 0.002-168Ω. This study provides a new approach for the development of efficient electrocatalyst for large-scale application in fuel cells.

Enhancing Water Splitting Photoanodes with Plasmonic Metal Nanoparticles

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Sunlight-driven photocatalysis is typically limited to the absorption of light with energy larger than the band gap of the chosen semiconductor photoabsorber. Significant portions of the solar spectrum, therefore, are lost when earth-abundant metal oxide photocatalysts including titanium dioxide, hematite, or copper oxides are used for reactions such as water splitting.

Plasmonic metal nanoparticles offer a route to the utilisation of sub-band gap energy photons incident on photoabsorbers. Depending on the composition, size and shape of these nanoparticles, low energy photons can be absorbed and form localised surface plasmon resonances. When situated in close proximity to a photocatalyst, these plasmons may then undergo plasmon-induced resonant energy transfer to create new excited electron-hole pairs within the photocatalytic material.¹ These newly excited charge carriers are in addition to those created upon light absorption by the semiconductor photocatalyst, leading to the possibility of surpassing theoretical maximum solar conversion efficiencies.

In this work, ambient-pressure, aerosol-assisted chemical vapour deposition is used to fabricate palladium nanoparticles on fluorine-doped tin oxide (FTO)-coated glass underneath coatings of bismuth vanadate (BiVO₄) visible light absorbing, earth-abundant photocatalyst for the oxygen evolution half-reaction of water splitting. BiVO₄ has a maximum solar-to-hydrogen conversion efficiency of 9.2% when only considering absorption of photons up to its bandgap, 2.4 eV in energy. This performance may not be competitive with photovoltaic-coupled electrolysis for commercialisation,² and therefore BiVO₄ is a strong candidate for enhancing with plasmonics.

Acknowledgements: A.K. thanks the EPSRC for a Programme Grant (Grant No. EP/W017075/1) and B.T. thanks the Catalysis Meets Plasmonics - CPLAS research programme for funding his postdoctoral research.

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2. B. Tam, O. Babacan, A. Kafizas, J. Nelson, *Energy Environ. Sci.*, **2024**, 17, 1677.



Tuning Interlayers spacing in layered oxide materials for high intercalated pseudocapacitive charge storage

Dr. Pravin Walke¹, Aruna Ivaturi², Harishchandra Nishad¹

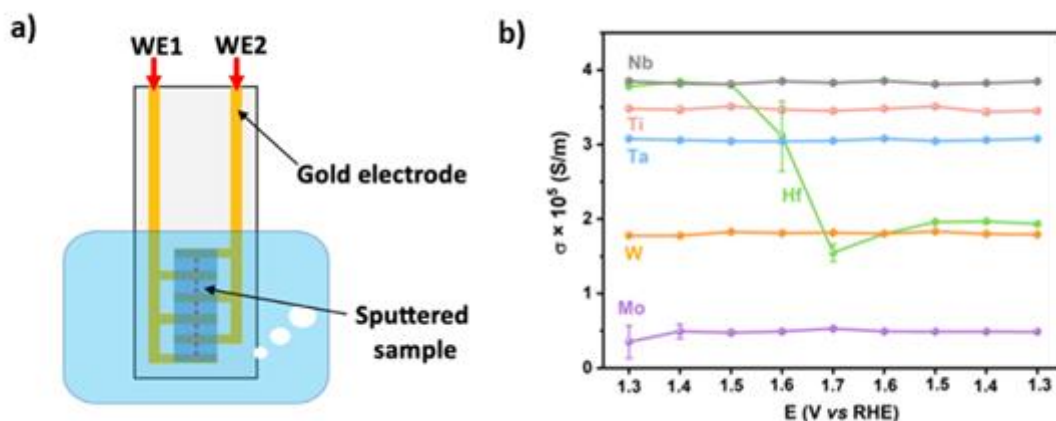
¹National Centre For Nanoscience's And Nanotechnology, University Of Mumbai, India, ²University of Strathclyde, United Kingdom

Layered double hydroxides (LDHs) can adopt superior conductivity and a charge-storage capacity due to the remarkable adjustability of layers. However, tuning of layers spacing in LDHs is a major challenge as it suffers from stacking issues, structural degradation, and issues with interstitial ion insertion. Here an effective strategy of exchanging interlayer ions within laminates was efficiently realized. Despite the layered spatial structure and morphological perturbation, the exchange of carbonate ions by sulfate anions into the interlayers of the NiFe-LDHs nanostructure exhibited an expansion of the layer spacing and rapid ion intercalation. A three-fold enhancement of the specific capacitance in NiFe-LDHs with sulfate anions (NFS), i.e. 527 F g⁻¹, was achieved over NiFe-LDHs with carbonate anions (NFC), at 0.5 A g⁻¹ in 6 M KOH aqueous electrolyte. Further, the aqueous hybrid supercapacitor (AQHS) of NFS-LDHs nanoplates displayed a high specific capacitance of 30 F g⁻¹ at 0.5 A g⁻¹, with a high energy density of 11 W h kg⁻¹ and a power density of 5500 W kg⁻¹. It eventually exhibited a tremendous capacitance retention of 83 % at 3 A g⁻¹ with a coulombic efficiency of 82% at up to 10 000 cycles. Thus the expansion of the layer spacing resulted in enhanced ionic intercalation, and improved conductivity and redox activity, underscoring the potential of NFS-based LDHs for advancing the performance of aqueous hybrid supercapacitors.

Probing in situ conductivity changes of supports for iridium oxide water oxidation electrocatalyst with the interdigitated electrodes

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Green hydrogen plays a key role in the transition to a sustainable low-carbon energy system. Proton exchange membrane water electrolysis (PEMWE) has been identified as the most promising green hydrogen production technology owing to its fast start-up and shut-down dynamics to be coupled with the intermittent renewable energy sources. However, the scarcity of the electrocatalyst, iridium, is the bottleneck of large-scale implementation of the PEMWE, where high loading of iridium oxide is used to catalyse the oxygen evolution reaction (OER) as well as to sustain an integrated conductive layer due to its incomparable activity and stability under the corrosive and oxidative OER conditions. Decades of annual production of iridium will be required to meet the global energy demand on a terawatt scale. The loading of iridium can be reduced by introducing a catalyst support. However, most metals suffer from conductivity loss when forming the oxide layers and these semi-conducting oxide layers are detrimental for the electron transfer in the PEMWE. Interdigitated array electrodes (IDEs) enable the real-time observation of the conductivity changes with two working electrodes of a 10-mV potential difference. Herein, we applied the IDEs to probe the conductivity loss of the early transition metals (Ti, Hf, Ta, Nb, Mo and W) under the OER conditions and assessed their capabilities of supporting iridium oxide water oxidation catalysts. Our preliminary results showed that Ti, Nb and Ta have sustained the conductivity under the OER conditions which made them promising candidates to support iridium oxide in the PEMWE.



Poster Presentations

Poster No.	First Name	Last Name	Organisation	Paper Title
1	Onajite Theresa	Abafé Diejomaoh	University Of Bristol, Bristol Composite Institute	Gel electrolytes based on cellulose acetate and a high lithium concentration phosphonium ionic liquid for high performing lithium-ion batteries
2	Mina	Ardani		Exsolution of Ultrasmall Pt Nanoparticles on High-Surface Area Mesoporous Assemblies of La _{0.985} Ba _{0.015} Al _{0.99} Pt _{0.01} O ₃ /Al ₂ O ₃ Towards Superior Selective Catalytic Oxidation of Ammonia
3	Nilanthy	Balakrishnan	Keele University	Symmetric double-layer capacitor with natural rubber and sodium salt-based solid polymer electrolyte and reduced graphene oxide electrodes
4	Habibat	Chahul	University of Cambridge	Corrosion Behaviour of the Zinc Anode in Aqueous Zinc-ion Batteries (Poster Presentation)
5	George	Creasey	Imperial College London	Up-scaling photoelectrochemical reactors – lab-scale optimisation to outdoor field testing
6	Will	Dawson		Predicting Crack Formation in Drying Slurry Cast Electrodes with In Situ X-ray CT
7	David J	Dunstan	Queen Mary University of London	Reappraisal of paths to decarbonising GB electricity generation in 2030
8	Mahwash Mahar	Gul	University of Birmingham	Lithium-ion high power cell: Lithiumwerks 26650 Battery Parameterization
9	Yi-Teng	Huang		A study on the optoelectronic properties of an emerging perovskite-inspired material - NaBiS ₂
10	G M Sadrul	Islam	Simap Lab, Cnrs-uga	Lithium Ionic Conductors from the Li ₃ PS ₄ -Li ₄ SiS ₄ Binary Thio-LISICON System
11	Ramsha	Khan	University of Surrey	Optimization of Powdered NiMo Electrocatalysts for Hydrogen Evolution Reaction: Influence of pH and Ni Composition
12	Capucine	Mamak	University of Cambridge	Investigating the impact of mechanical strain on the optoelectronic properties of metal halide perovskites in four dimensions
13	Kinga	Mastej	Imperial College London	Semiconducting Materials from Analogy and Chemical Theory
14	Louise	Oldham	Imperial College London	Spectroscopic insights into the electrochemical origins of quasi-Fermi level splitting in Fe ₂ O ₃ photoanodes
15	Manoj	Ovhal	University of Birmingham	Investigation of Ion Solvation on Sodium-ion Diffusivity in Hard Carbon
16	Aparna	Parakkad Unnikrishnan	University of Surrey	COMPUTATIONAL INVESTIGATION OF CALENDERING EFFECTS ON ELECTRODE STRUCTURE AND PERFORMANCE USING DISCRETE ELEMENT METHOD
17	Aritra	Roy	London South Bank University	ComProScanner: A multi-agent based agile framework for high quality composition-property structured data extraction from scientific literature
18	Kezia	Sasitharan	Newcastle University	Powering the Future: Metal-Organic Nanosheets for Integrated Solar Energy Capture and Storage
19	Tayyaba	Shahzadi		Synergistic effect of trimetallic SnBiCu nanoparticles decorated on graphene oxide as high efficient electrocatalyst for fuel cell application
20	Brian	Tam	Imperial College London	Enhancing Water Splitting Photoanodes with Plasmonic Metal Nanoparticles
21	Pravin	Walke	National Centre For Nanoscience's And Nanotechnology, University Of Mumbai	Tuning Interlayers spacing in layered oxide materials for high intercalated pseudocapacitive charge storage
22	Meimei	Yang	Imperial College London	Probing in situ conductivity changes of supports for iridium oxide water oxidation electrocatalyst with the interdigitated electrodes

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