

# Worcester Energy Day 2024

21 February 2024

13:00 - 18:00

Sultan Nazrin Shah Centre, Worcester College

## PROGRAM & BOOK OF ABSTRACTS



13:00 - 13:15	Arrival & Registration	
13:15 - 13:20	Welcome address by Sustainability Fellow of Worcester College (Prof. Lisa Wedding)	
Plenary Talks (Chair: Dr. Krishanu Dey)		
13:20 - 13:45	Prof. Henry Snaith	Emergence Of Halide Perovskites for Photovoltaics and Lighting Applications
13:45 - 14:10	Prof. Robert Hoyer	Sustainable Bismuth-Based Materials for Photovoltaics and Solar Fuels
14:10 - 14:35	Prof. Paul Shearing	Engineering Net Zero: The Role of Energy Storage
14:35 - 14:40	Comfort break	
Oral Presentation Session 1 (Chair: Dr. Krishanu Dey)		
14:40 - 14:48	Dr. Pascal Kaienburg	Evaporated organic solar cells – materials, structure, function
14:48 - 14:56	Dr. Nicola Courtier	Electrochemical modelling of lithium-ion batteries and perovskite solar cells
14:56 - 15:04	Esther Yi-Hang Hung	A novel, lead-free halide perovskite derivative for ferro- and piezo-electric applications
15:04 - 15:12	Lennart Baumgärtner	Renewable Economy: what the data tells us
15:12 - 15:20	Shaoni Kar	Dimethylammonium-incorporated mixed halide perovskite nanocrystals for stabilized red emission
15:20 - 15:28	Gayatri Sundar Rajan	Development of Water & Cooling Cogeneration System for the Water-Energy-Food Nexus
15:28 - 15:36	Jack Palmer	Shedding light on organic photovoltaics: How electron spin resonance can help us understand the photovoltaic mechanism
15:36 - 15:44	Rahul Ajit Nambiar	Scalable route to all vacuum processed perovskite solar cells
15:45 - 16:35	Poster Presentation & Networking	
Oral Presentation Session 2 (Chair: Dr. Krishanu Dey)		
16:35 - 16:43	Dr. Junzhi Ye	Direct linearly-polarised electroluminescence from colloidal perovskite nanoplatelet superlattices
16:43 - 16:51	Dr. Noël Halleman	Characterising lithium-ion batteries with operando electrochemical impedance spectroscopy
16:51 - 16:59	Zi Huang	A synergistic system of carbon capture and hydrogen production with waste heat recovery for industrial decarbonization
16:59 - 17:07	Akash Dasgupta	Visualizing Macroscopic Inhomogeneities in Perovskite Solar Cells
17:07 - 17:15	Rohit Rungta	Minimising Membrane Fouling in the Non-aqueous Vanadium Acetylacetonate Redox Flow Battery
17:15 - 17:23	Omar Daoud	Green Cement Production from Seawater to Mitigate CO <sub>2</sub> Emissions
17:23 - 17:31	John Cattermull	Prussian Blue Analogue Cathodes for Fast-Charging K-ion Batteries
17:31 - 17:39	Florine Rombach	Material and device stability of lead-tin perovskite solar cells
17:39 - 17:47	Honora Driscoll	Green ammonia production using tidal stream energy in the UK
17:50 - 17:55	Closing remarks by Head of Research of Worcester College (Prof. John Parrington)	
17:55 - 18:00	Delegates leave	

## List of Plenary Speakers

### 1. Professor Henry Snaith FRS

Binks Professor of Renewable Energy, Department of Physics, University of Oxford  
Co-founder & Chief Scientific Officer, Oxford PV  
Co-founder, Board Director & Chief Scientific Officer, Helio Display Materials

Group website: <https://www.physics.ox.ac.uk/research/group/photovoltaic-and-optoelectronic-device-group>

### 2. Professor Robert Hoyer

Associate Professor of Inorganic Chemistry, Department of Chemistry, University of Oxford  
Tutorial Fellow, St John's College, University of Oxford  
Chief Technology Officer, NanoPrint Innovations Ltd.

Group website: <https://hoyegroup.web.ox.ac.uk/>

### 3. Professor Paul Shearing

Professor of Sustainable Energy Engineering, Dept. of Engineering Science, University of Oxford  
Royal Academy of Engineering Chair in Emerging Battery Technologies  
Director, ZERO Institute, University of Oxford

Website: <https://eng.ox.ac.uk/people/paul-shearing/>

## List of Poster Presentations

Jasper Singh	Expanding the Electrochemical Stability Window of Aqueous Electrolytes in Li-ion batteries
Dr. Yi-Teng Huang	NaBiS <sub>2</sub> as an emerging photovoltaic absorber?
Qimu Yuan	All-vacuum-processed Perovskite Solar Cells with Excellent Thermal Stability
Freddie Leslie	Mixed Conductivity Polymers for Multifunctional Electrode Binders
Galen Brown	Novel manufacturing approaches for smarter Na-ion cathodes
Dr. Liam Bird	Operando Raman mapping at the cathode/ electrolyte interface in lithium-sulfur cells
Kieran Stakem	Non-Conjugated Conducting Polymers for Energy Storage Application

# List of Abstracts for Oral Presentations

## Oral Presentation Session 1

14:40 - 14:48 [Dr. Pascal Kaienburg \(Department of Physics\)](#)

### **Evaporated organic solar cells – materials, structure, function**

Vacuum-thermal-evaporation (VTE) of small semiconducting molecules has advantages over wet-chemical deposition when it comes to commercializing organic electronics technologies as exemplified by OLEDs and organic photovoltaics (OPV). Advantages include homogeneous film growth over large areas and using molecules with defined molecular weight and advanced purification protocols. In the context of OPV, a less-explored molecule design space and lacking control over microstructure constitute the main drawbacks of VTE compared to solution processing.

Here, we study various state-of-the-art VTE OPV systems, such as oligothiophene blends with C60, to quantify performance strength and drawbacks of the currently available molecules. We characterize the devices in terms of voltage loss, absorption strength and mobility with sensitive photocurrent spectroscopy, ellipsometry, and transient charge extraction, respectively. These optoelectronic properties will depend on the way the molecules arrange in a thin film. We thus investigate processing-microstructure relations by varying the substrate temperature during deposition and characterize phase separation and crystallinity with resonant soft X-ray scattering (RSoXS) and wide-angle (hard) X-ray scattering (WAXS), respectively. Finally, we demonstrate the benefit of a novel class of molecules, so-called non-fullerene acceptors, for VTE OPV – highlighting the enormous potential for interdisciplinary molecule development between device physicists, synthetic chemists, and computational material designers.

14:48 - 14:56 [Dr. Nicola Courtier \(Department of Engineering Science\)](#)

### **Electrochemical modelling of lithium ion batteries and perovskite solar cells**

Renewable energy generation and storage technologies are vital for the global transition to clean energy. Both batteries and solar panels are typically comprised of cells, connected to form modules which in turn are connected to form solar arrays or battery packs. These devices rely on the electrochemical processes occurring within each cell. I use modelling and simulation to study cell behaviour. My research aims to understand how we can design more efficient and longer-lasting cells, by identifying pathways to degradation.

Electrochemical modelling is challenging due to the complex interactions which occur between ionic and electronic species in devices such as lithium-ion batteries and perovskite solar cells. Once a cell is made, only external measurements can be taken and internal mechanisms must be inferred from them. I am developing parameterisation methods to identify changes in the underlying material properties from just voltage, current and temperature data. I will show how my open-source software has been used to investigate ion migration in perovskites, capacity fade in lithium-ion batteries and health-aware fast-charging protocols.

14:56 - 15:04 [Esther Yi-Hang Hung \(Department of Physics\)](#)

### **A novel, lead-free halide perovskite derivative for ferro- and piezo-electric applications**

Ferroelectricity is the phenomena of spontaneous electric polarization  $P_s$  which is reversible under an external electric field. All ferroelectric materials also exhibit piezoelectricity; strain-induced electric polarization or conversely, electric-field induced strain. Applications include sensors, actuators, transducers and vibrational energy harvesters. Molecular ferroelectrics have recently attracted interest over traditional ceramics due to simpler processing methods, their light-weight nature and mechanical flexibility. Here, we study the ferroelectric properties of a novel organic-inorganic material which displays potential for being used as a piezoelectric energy harvester, or even for piezo-photovoltaic applications via the bulk photovoltaic effect.

15:04 - 15:12 [Lennart Baumgärtner \(Department of Geography\)](#)

### **Renewable Economy: what the data tells us**

Technological change and innovation are a vital part of the energy transition. In the electricity sector, clean generation technologies such as renewables must replace fossil fuel technologies within the next decades. This constitutes a significant, non-marginal change in our technology landscape. What can previous technological change stories tell us about the renewable future? It turns out that there are some remarkable patterns in technological evolution. Particularly in the economics of technological change, these patterns are highly predictable and consistent.

For this talk, we will look at historical patterns of technological change and innovation. Based on these observations, we can make quantitative predictions of future changes in the renewable economy. In particular, we will look at how fast we can ramp up global renewables and what costs are associated to this transition. We compare different technological solutions to the energy transition and discuss how quantitative models can help navigate the transition.

15:12 - 15:20 [Shaoni Kar \(Department of Physics\)](#)

### **Dimethylammonium-incorporated mixed halide perovskite nanocrystals for stabilized red emission**

In addition to their stellar performance in photovoltaics, metal halide perovskites have seen outstanding performance in light emission applications. With high exciton binding energies affording enhanced quantum confinement of carriers, inorganic perovskite nanocrystals (NC) have proved to be superior candidates for realizing colour-pure, highly efficient light emitting diodes (LEDs) owing to their easy bandgap tunability through compositional engineering, narrow emission peaks and high photoluminescence quantum yields. In this work, we present a novel room-temperature synthesis to alloy the A-site of pure-red emitting CsPbI<sub>2</sub>Br NCs with dimethylammonium (DMA) to improve its phase stability under excitation while retaining high photoluminescence quantum yields. To our knowledge, this is the first study of DMA-alloying through facile ligand assisted reprecipitation (LARP) synthesis techniques. We propose a novel synthetic route at room temperature and then study the crystal structure and morphology as a function of different DMA contents through an interplay of crystallographic and optical data. We report higher ambient stability even under intense optical excitation. Finally, we employ these materials as the emitter layer in LEDs and find significant improvement in LED performances with notably improved air-stability in the DMA-incorporated variant.

15:20 - 15:28 [Gayatri Sundar Rajan \(Department of Engineering Science\)](#)

### **Development of Water & Cooling Cogeneration System for the Water-Energy-Food Nexus**

At the water-energy nexus, evaluating synergies between desalination and refrigeration processes offers an opportunity to reduce the energy consumption of two traditionally energy-intensive processes. Adsorption desalination and cooling (ADS) cogeneration systems present an alternative to traditional desalination systems in that they feature no moving parts, enable double distillation, and are driven by low-grade heat sources. When coupled with humidification-dehumidification (HDH) systems, the ADS-HDH system can produce higher efficiency and lower cost water and cooling than standalone alternatives.

To investigate the coupled ADS-HDH system, this study uses a lumped parameter numerical ADS model and a black box numerical model of the HDH system, both written in MATLAB. The purpose of the simulation is to determine the threshold of operating conditions that improve combined system performance. Preliminary results highlight an increase in Gain Output Ratio, metric for thermal desalination efficiency, and Energy Utilization Factor, a metric that highlights the efficiency of a coupled system vs standalone alternatives.

This oral presentation will highlight results of the ADS-HDH model, discuss the flow of energy throughout the system, and highlight key applications of the technology. The purpose of this presentation is to spotlight opportunities to innovate in sustainable development at the water-energy-food nexus.

15:28 - 15:36 [Jack Palmer \(Department of Chemistry\)](#)

## **Shedding light on organic photovoltaics: How electron spin resonance can help us understand the photovoltaic mechanism**

In the last decade, organic photovoltaics (OPVs) have shown remarkable advances in efficiency and lifetime and are already finding initial commercial applications. One of their biggest advantages is tunability, allowing for control of colour, transparency, and flexibility. The notable success of new types of acceptor materials, enabling higher power conversion efficiencies, has renewed interest in the details of the photovoltaic mechanism. Since the states involved in the mechanism - charge-transfer states, separated charges, and triplet states - are all paramagnetic, they can be characterised by electron spin resonance (ESR) spectroscopy.

By using the spins as probes, ESR can provide complementary information to widely used optical characterisation techniques. In particular, the formation mechanism of photoinduced paramagnetic states is encoded in the observed spin polarisation of ESR spectra, a result of non-equilibrium population distributions. Based on the spin polarisation, ESR can distinguish between singlet- and triplet-born charge-transfer states, as well as between intersystem crossing and geminate recombination triplets.

In this talk, I will present an investigation of both fullerene- and non-fullerene-based OPVs using ESR spectroscopy. Paramagnetic states generated following photoexcitation are characterised, and the evolution of the spin states with time is examined to identify differences in spin dynamics between different materials.

15:36 - 15:44 [Rahul Ajit Nambiar \(Department of Physics\)](#)

## **Scalable route to all vacuum processed perovskite solar cells**

Vacuum deposition has recently emerged as a pivotal technique for scaling up perovskite solar cells (PSCs) in commercial applications, offering advantages of conformal coating and controlled layer thickness, thereby aligning with large-scale manufacturing needs. In this regard, process optimization during batch-to-batch fabrication is imperative for consistent and efficient PSC production. Atmospheric conditions, particularly moisture in the form of relative humidity, significantly impact perovskite layer quality, necessitating controlled environments. Through in-situ grazing incidence wide angle x-ray diffraction (GIWAX) and 3D time of flight secondary ion mass spectroscopy (ToF-SIMS), we show that annealing in the presence of humidity is essential for the intermixing of organic and inorganic precursors necessary to achieve high quality thermally evaporated perovskite absorbers via sequential deposition. Notably, spectroscopy measurements also indicate a bulk limitation in the photoluminescence efficiencies of absorbers when processed without the presence of any relative humidity, bolstering the importance of controlled humidity for improved device performance. This breakthrough has resulted in the development of high-performance methylammonium-free PSCs exclusively processed through vacuum techniques, achieving an impressive power conversion efficiency of 20.45%, which is one of the highest efficiencies reported for all-evaporated PSCs. Ageing these devices under open circuit at 85 °C and 1 sun illumination reveals remarkable stability for more than 500 hours, although an initial burn-in phase is observed in the beginning. This finding highlights the potential of vacuum deposition as a viable method to obtain high performance perovskite devices.



## Oral Presentation Session 2

16:35 - 16:43 [Junzhi Ye \(Department of Chemistry\)](#)

### **Direct Linearly-polarised Electroluminescence from Colloidal Perovskite Nanoplatelet Superlattices**

Polarised light is critical for a wide range of applications, but is usually generated by filtering unpolarised light, which leads to significant energy losses and requires additional optics. Herein, the direct emission of linearly-polarised light is achieved from light-emitting diodes (LEDs) made of CsPbI<sub>3</sub> perovskite nanoplatelet superlattices. Through use of solvents with different vapour pressures, the self-assembly of perovskite nanoplatelets is achieved to enable fine control over the orientation (either face-up or edge-up) and therefore the transition dipole moment. As a result of the highly-uniform alignment of the nanoplatelets, as well as their strong quantum and dielectric confinement, large exciton fine-structure splitting is achieved at the film level, leading to pure-red LEDs exhibiting a high degree of linear polarisation of 74.4% without any photonic structures. This work unveils the possibilities of perovskite nanoplatelets as a highly promising source of linearly-polarised electroluminescence, opening up the development of next-generation 3D displays and optical communications from this highly versatile, solution-processable system.

16:43 - 16:51 [Noël Hallemons \(Department of Engineering Science\)](#)

### **Characterising lithium-ion batteries with operando electrochemical impedance spectroscopy**

"Reaching net zero by 2050 requires improved battery manufacturing and usage. A crucial point to improve is battery characterisation, e.g. characterising the performance of novel chemistries and monitoring state-of-health along their lifetime.

Ideally, this should be done noninvasively. To this aim, there are three quantities that can easily be accessed: current, voltage, and temperature. Impedance spectroscopy is often applied to characterise batteries from current and voltage data. The frequency-dependent impedance provides information on electrochemical processes happening at different time scales, for instance diffusion and charge transfer. However, a major drawback is that it can only be applied to batteries in equilibrium. And, hence, not to batteries during operation (charging/discharging).

In this research, we developed a tool to characterise batteries in operating conditions. We leverage multisine excitations to unravel how the impedance changes over time. We show advantages of characterising batteries in operating conditions and provide examples of applications.

The presentation will consist of the simplified results given in the following publication.

Hallemons, N., Howey, D., Battistel, A., Saniee, N.F., Scarpioni, F., Wouters, B., La Mantia, F., Hubin, A., Widanage, W.D. and Lataire, J., 2023. Electrochemical impedance spectroscopy beyond linearity and stationarity—A critical review. *Electrochimica Acta*, p.142939."

16:51 - 16:59 [Zi Huang \(Department of Engineering Science\)](#)

### **A synergistic system of carbon capture and hydrogen production with waste heat recovery for industrial decarbonization**

This project aimed at solving the high energy demand and cost issue in industrial decarbonization by addressing a synergistic system of Calcium Looping (CaL) and Dry Reforming of Methane (MDR) which was designed to recover the exhausted heat from flue gas simultaneously. CaL captured CO<sub>2</sub> from the industrial flue gases through the carbonation reaction of CaO. Then, CO<sub>2</sub> was released through the calcination reaction of CaCO<sub>3</sub> and was fed for MDR to produce hydrogen. Meanwhile, the high-grade heat recovered by CaL from flue gas provided heat demand for MDR. Obviously, such a synergistic process can potentially improve the energy efficiency and achieve a circular carbon economy.

16:59 - 17:07 [Akash Dasgupta \(Department of Physics\)](#)

## **Visualizing Macroscopic Inhomogeneities in Perovskite Solar Cells**

Despite the incredible progress made, the highest efficiency perovskite solar cells are still restricted to small areas (<1 cm<sup>2</sup>). In large part, this stems from a poor understanding of the widespread spatial heterogeneity in devices. Conventional techniques to assess heterogeneities can be time consuming, operate only at microscopic length scales, and demand specialized equipment. We overcome these limitations by using luminescence imaging to reveal large, millimetre-scale heterogeneities in the inferred electronic properties. We determine spatially resolved maps of “charge collection quality”, measured using the ratio of photoluminescence intensity at open and short circuit. We apply these methods to quantify the inhomogeneities introduced by a wide range of transport layers, thereby ranking them by suitability for upscaling. We reveal that top-contacting transport layers are the dominant source of heterogeneity in the multilayer material stack. We suggest that this methodology can be used to accelerate the development of highly efficient, large-area modules, especially through high-throughput experimentation.

17:07 - 17:15 [Rohit Rungta \(Department of Engineering Science\)](#)

## **Minimising Membrane Fouling in the Non-aqueous Vanadium Acetylacetonate Redox Flow Battery**

Due to their unique advantages in long cycle lives and modular designs, redox flow batteries (RFBs) are being developed to peak shave energy from intermittent sources. RFBs have yet to meet the cost requirements needed to achieve broad market penetration, however. The second largest cost of RFBs is the ion-exchange membrane, accounting for 30% of the total cost. Porous separators provide a pathway to decrease the cost of RFBs, but long-term performance has been difficult to assess due to the coupling of electrolyte degradation, self-discharge, and membrane fouling.

A novel set of ‘canary cell’ experiments unequivocally point to membrane fouling as the predominant factor that drives permanent cell degradation in the V(acac)<sub>3</sub> RFB. An adaptive observer is used to monitor the crossover rate during self-discharge experiments. The porous separators start off with ideal Fickian behavior because crossover is a linear function of the state of charge. Over time, however, the cell deviates, with active-species crossover becoming non-Fickian as the membrane fouls. It is hypothesized that pore clogging is responsible for this decreasing mass transfer coefficient, and in turn fading cell performance. Deconvoluting membrane and electrolyte processes is crucial to determine the stability and long-term viability of RFB electrolyte systems.

17:15 - 17:23 [Omar Daoud \(Department of Engineering Science\)](#)

## **Green Cement Production from Seawater to Mitigate CO<sub>2</sub> Emissions**

Concrete production emits 8% of global carbon emissions. By valorizing brine from desalination to create concrete, we can decarbonize one of the world’s most heavily carbon-intensive industries. Through exchanging traditional cement materials (calcium carbonate, CaCO<sub>3</sub>) with a seawater-derived alternative (magnesium hydroxide, MgO-based option), we can capture CO<sub>2</sub>, reduce the energy intensity of the cement industry, and maintain the quality of created cement.

The process uses the discharged brine from desalination plants as the only feedstock to produce a strong base (NaOH). The brine is then recycled to induce Mg<sup>2+</sup> precipitation in the form of Mg(OH)<sub>2</sub>. Unlike CaCO<sub>3</sub>, MgO-based cement can be calcinated at lower temperatures (500 °C), reducing the processes’ energy consumption, and only releases water vapor as a byproduct.

In my presentation, I will highlight the potential of the process to reduce the cost per unit of carbon captured compared to Direct Air Capture by five times (35.7 \$/t<sub>CO<sub>2</sub></sub> vs 180 \$/t<sub>CO<sub>2</sub></sub>), reduce the energy consumption of existing cement production, and valorize brine from desalination plants.



17:15 - 17:23 [John Cattermull \(Department of Materials/Chemistry\)](#)

### **Prussian Blue Analogue Cathodes for Fast-Charging K-ion Batteries**

Potassium-ion batteries (KIBs) are gaining attention as a viable complementary technology to lithium-ion batteries, attributed to their anticipated cost-effectiveness and high-rate capabilities. In my presentation, I will discuss the progress we have made in understanding the structure-electrochemistry relationship of Prussian Blue analogue cathodes. Additionally I will discuss their performance within a K-ion battery, evaluating their potential for facilitating rapid charging.

17:23 - 17:31 [Florine Rombach \(Department of Physics\)](#)

### **Material and device stability of lead-tin perovskite solar cells**

Tripling renewable energy production capacity by 2030 will necessitate energy sources which can be made cheaply and quickly from abundant materials. Perovskite multi-junction solar cells, which normally utilize mixed lead-tin perovskites for the bottom absorber, are a promising candidate. However, solar cells based on mixed lead-tin perovskites tend to suffer from poor stability under operating conditions.

We explore the causes of this instability under extended periods of combined 65°C thermal and illumination stressing using a range of structural, optical, and electronic characterization techniques on lead-tin perovskite films, half-stacks and devices. We show that the bulk phase and optoelectronic quality of lead-tin perovskite films are stable on timescales that exceed those of device degradation and demonstrate through device simulations that the small changes observed can only account for a minor portion of the observed device degradation.

We find instead that the observed behaviour of the device can fully be explained by considering an increasing impact of mobile ions during aging, which we demonstrate to be the major cause of early-time performance loss. Ultimately, we show that the mitigation of the impact of mobile ions can make lead-tin perovskites significantly more stable and demonstrate this with an alternate device stack.

17:23 - 17:31 [Honora Driscoll \(Department of Engineering Science\)](#)

### **Green ammonia production using tidal stream energy in the UK**

Ammonia is the second most-produced chemical in the world, but it is currently primarily produced using natural gas. However, ammonia can be produced using renewable energy - this is called green ammonia. Proposed green ammonia plants focus primarily on solar and wind energy, both of which are intermittent sources of energy. The ammonia production process benefits from a constant energy source, to avoid expensive energy storage. Tidal stream energy is a predictable and largely unexploited energy source. This presentation looks at the potential of tidal stream energy for green ammonia in the UK and explains its benefits.

## **List of Abstracts for Poster Presentations**

[Jasper Singh \(Department of Materials\)](#)

### **Expanding the Electrochemical Stability Window of Aqueous Electrolytes in Li-ion batteries**

With the adoption of intermittent renewable energy supplies and the growing markets of electric vehicles and portable/wearable consumer electronics; the demand for electrochemical energy storage devices has increased. Aqueous electrolyte Li-ion batteries are now a promising battery candidate owing to their low cost, enhanced safety, and high ionic conductivity. However, their narrow Electrochemical Stability Window (ESW) due to water decomposition has so far impeded their commercial use. Subsequent experiments have shown that the ESW greatly expands as a result of Water-In-Salt electrolytes (WISEs) decomposing and forming a passivating layer on the electrode. Furthermore, the work showcased in this poster reveals how different solute-solvent interactions affect water activity and allow for highly stable water-based electrolytes to be used with a broad range of electrodes, therefore improving the energy density of aqueous Li-ion batteries.

[Dr. Yi-Teng Huang \(Department of Chemistry\)](#)

### **NaBiS<sub>2</sub> as an emerging photovoltaic absorber?**

I-V-VI<sub>2</sub> ternary chalcogenides (ABZ<sub>2</sub> materials) are gaining attention as earth-abundant, nontoxic, and air-stable absorbers for photovoltaic applications. However, the materials explored thus far have slowly-rising absorption onsets, and their charge-carrier transport is not well understood yet. In this work, we investigate the photovoltaic potential of NaBiS<sub>2</sub> nanocrystals, which have a steep absorption onset, with absorption coefficients reaching  $>105 \text{ cm}^{-1}$  just above its pseudo-direct bandgap of 1.4 eV. Surprisingly, we also observe an ultrafast (picosecond-time scale) photoconductivity decay and long-lived charge-carrier population persisting for over one microsecond in NaBiS<sub>2</sub> nanocrystals. These unusual features arise because of the presence of non-bonding S p states just above the upper valence band, which is facilitated by cation disorder. We also revealed that although the strong absorption strength of NaBiS<sub>2</sub> enables the fabrication of its ultrathin devices, the strong charge-carrier localization along with ion migration still limit the efficiencies of NaBiS<sub>2</sub> solar cells. Therefore, future efforts on improving photovoltaic performance of NaBiS<sub>2</sub> solar cells should be focussed on tuning cation disorder and suppressing ion conductivity.

[Qimu Yuan \(Department of Physics\)](#)

### **All-vacuum-processed Perovskite Solar Cells with Excellent Thermal Stability**

In this work, we investigated organometallic copper phthalocyanine (CuPc) and zinc phthalocyanine (ZnPc), deposited via the thermal-evaporation method, as alternative, low cost, and durable hole transport layers (HTLs) in all-vacuum-deposited solvent-free [CH(NH<sub>2</sub>)<sub>2</sub>]<sub>0.83</sub>CS<sub>0.17</sub>PbI<sub>3</sub> (FACsPbI<sub>3</sub>) perovskite solar cells. We revealed that the CuPc HTL demonstrated improved compatibility in a p-i-n photovoltaic device, in comparison with ZnPc. Furthermore, we thoroughly examined the long-term stability of these all-vacuum-processed devices under a range of testing conditions. Importantly, unencapsulated devices as large as 1 cm<sup>2</sup> exhibited outstanding thermal durability, demonstrating no observable degradation in efficiency after more than 5000 hours in storage and 3700 hours under 85 °C heat-stressing in N<sub>2</sub> atmosphere. In addition, we uncovered the striking differences in the sticking, adhesion, and nucleation dynamics of the organic perovskite precursor, formamidinium iodide (FAI), to various HTLs. Therefore, we highlight the impact of varying sticking characteristics to the stoichiometry of the formed perovskite thin films from co-evaporation. We believe that this finding epitomises the importance of optimising growth parameters specific to individual charge transport layer if FAI is to be used as a precursor in any co-evaporated perovskite.

[Freddie Leslie \(Department of Chemistry\)](#)

### **Mixed Conductivity Polymers for Multifunctional Electrode Binders**

Electric vehicles and modern electronics require increasingly high capacities and potentials in lithium ion batteries, and the current state of the art is insufficient to meet demand. One major barrier to this is the polymer typically used as an electrode binder, poly(vinylidene fluoride), which lacks useful ionic and electronic conductivities, as well as having poor mechanical and adhesion properties for modern electrodes. Our work is in creating new polymers which tackle these issues, to improve battery cyclabilities and capacities. We have been focussing on the synthesis of ABA block copolymers, where the A block is electronically conductive and the B block is ionically conductive. Electronic conductivity allows electrons to transport from the cathode to the current collector, removing the need for conductive additives. The ionically conductive block allows for improved lithium transport, lowering internal resistance, as well as improving adhesion to ceramic cathode materials. The different properties of the blocks lead to phase separation, which imparts elastomeric properties that are ideal for maintaining the integrity of electrodes, improving cyclability.

[Galen Brown \(Department of Materials\)](#)

### **Novel manufacturing approaches for smarter Na-ion cathodes**

Sodium-ion batteries (NIBs) are a promising alternative to their lithium counterparts (LIBs), which currently dominate electric vehicle and portable device applications. While NIBs have potential cost and safety advantages, they still lag behind LIBs in capacity, power output and longevity. There is therefore a drive to develop more energy-dense electrodes in order for NIBs to become commercially viable.

A possible route to higher energy density is increasing electrode thickness. However, this leads to a decrease in the maximum power output of the cell, as the transport of sodium ions is limited by diffusion. The resulting trade-off between the energy and power densities restricts the thickness of electrodes to  $\approx 60\text{-}90\ \mu\text{m}$ . Slurry casting, the most common electrode manufacturing process, places further practical limitations on thickness, and typically produces homogenous electrodes with little scope for structural variation.

This project aims to disrupt the trade-off between energy and power, developing novel manufacturing approaches to produce electrodes with heterogeneous structures. By slurry casting in multiple layers using different materials, the electrochemical behaviour can differ greatly from a homogenous single layer as charging/discharging rate is varied. These effects are investigated using well-established materials for sodium-ion cathodes.

[Dr. Liam Bird \(Department of Engineering Science\)](#)

### **Operando Raman mapping at the cathode/ electrolyte interface in lithium-sulfur cells**

Lithium-sulfur (Li-S) batteries are promising for applications in large-scale storage of renewable energy due to the low cost and abundance of sulfur, and for applications in aerospace due to their light weight. Attaining high cell-level capacity requires fabricating cathodes with high areal sulfur loading ( $> 5\text{mg}/\text{cm}^2$ ). However, it is necessary to ensure that sulfur is reversibly converted to/ from polysulfides (PS) throughout the cathode thickness, since the greater thickness ( $> 200\ \mu\text{m}$ ) due to higher areal loading can limit the Li-S cell's rate capability and reversible capacity. Spatially-resolved operando Raman spectroscopy is used here to characterise the electrochemical activity in the cathode, including the presence, distribution, and speciation of the active material and side-products formed during discharge/ charge. In this work, operando Raman line scans were paired with principal component analysis to provide real-time insights into electrochemical processes through the cross section of a Li-S cell, providing a starting point for future exploration of the effect of higher charge/ discharge rates and novel electrode architectures.

## **Non-Conjugated Conducting Polymers for Energy Storage Application**

Controlled polymerisation techniques, namely, ring-opening (co)polymerisation, are used to synthesise polyether and ester materials capable of conduction with the ultimate aim of developing mixed ionic-electronic conductors using redox-active and single-ion conducting polymers. Thermal and mechanical properties of the materials synthesised will be measured alongside conductivities and other properties relevant to the application. The use of polymers allows for control over the flexibility of the material, paving the way for applications in soft wearable electronics and flexible solid-state batteries.