# **Worcester Energy Day 2025**

28 February 2025 13:30 - 18:30 Sultan Nazrin Shah Centre, Worcester College

## PROGRAM & BOOK OF ABSTRACTS







13:15 - 13:35	Arrival & Registration		
13:35 - 13:45	Welcome address by the Sustainability Fellow of Worcester College		
	(Prof. Lisa Wedding)		
Plenary Talks (Chair: Dr. Krishanu Dov)			
13:45 - 14:10 Prof. Ruy Sebastian Bonilla Powering the Future with Silicon Solar Cells			
14.10 - 14.35	Prof. Radhika Khosla	Heat cooling and sustainable development	
14:35 - 15:00	Prof Moritz Riede	Organic Photovoltaics - What's next?	
15:00 - 15:05		Comfort break	
15:05 - 15:15	Presentation from the ZERO Institute		
Oral Presentation Session 1			
(Chair: Dr. Krishanu Dey)			
15:15 - 15:25	Dr. Theodore Hobson	Solar Cell Design for a Multi-Terawatt Future	
15:25 - 15:35	Dr. Yige Sun	Mapping Li Concentration Gradients across Battery Cathodes	
15:35 - 15:45	Robin Nicholson	Japan's Push for Hydrogen: Will it Work (this time)?	
15:45 - 15:55	Matthew Williams	Ultra-high surface area layered double hydroxide-based nanomaterials for sustainable chemistry	
15:55 - 16:05	Dr. Junzhi Ye	Extending the defect tolerance of halide perovskite nanocrystals to hot carrier cooling dynamics	
16:05-16:45		Tea/Coffee & Networking	
Flash Talks Session			
(Chair: Dr. Krishanu Dey)			
16:45 - 16:48	George Carew-Jones	Understanding routes to energy project bankability in Zambia	
16:48 - 16:51	Kanksshi agarwal	An analysis of relevant political narratives emerging in global south	
16:51 - 16.54	Karan Mukhi	Aggregation of Flexibility in Populations of Distributed Energy Resources	
16.54 - 16.57	Dr. Phil Grunewald	Observing and changing household energy use with better data, information and messages	
16.57 - 17.00	Marcel Seger	Firm level optimisation strategies for sustainable and cost- effective electric vehicle workplace charging	
17.00 - 17.03	Laurence Peinturier	The Role of Building Energy Simulation in Achieving Net-Zero Operating Emissions in the UK Non-Domestic Building Sector	
17.03 - 17.15		Overall Q&A and Discussion	
Oral Presentation Session 2			
(Chair: Dr. Krishanu Dey)			
17:15 - 17:25	Shaoni Kar	Evaporated inorganic perovskites for light emission	
17:25 - 17:35	Claire Torina Coulthard	Novel materials for CO <sub>2</sub> conversion: Challenges and opportunities	
17:35 - 17:45	Peter Akinshin	Hybrid processing of perovskite thin films for terawatt-scale photovoltaics	
17:45 - 17:55	Xiaohang Cai	Advancing Flexible Thermoelectric Generators for Wearable Energy Harvesting	
17:55 - 18:05	Haozhe Zhang	Tuning Layered Perovskite for Efficient Photocatalytic NH <sub>3</sub> Decomposition	
18.05 – 18.15	Lorenzo Catini	Exploring photophysical mechanisms in organic solar cells through electrically detected magnetic resonance	
18:15 - 18:20	Remarks by Dr. Michael Drolet FRHistS (SRF at Worcester College)		
18.20 - 18.25	Closing remarks by Head of Research of Worcester College (Prof. John Parrington)		
18:25 - 18:30	Delegates leave		
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### **List of Plenary Speakers**

#### 1. Professor Ruy Sebastian Bonilla

Associate Professor, Department of Materials, University of Oxford Tutorial Fellow, St. Anne's College

Group website: <a href="https://interface.materials.ox.ac.uk/home">https://interface.materials.ox.ac.uk/home</a>

#### 2. Professor Radhika Khosla

Associate Professor, Smith School of Enterprise and Environment, University of Oxford Research Director, Oxford India Centre for Sustainable Development, Somerville College Programme Leader in Zero Carbon Energy Use, ZERO Institute

Website: https://www.smithschool.ox.ac.uk/person/dr-radhika-khosla

#### 3. Professor Moritz Riede

Professor of Soft Functional Nanomaterials, Department of Physics, University of Oxford Governing Body Fellow, Wolfson College Co-Founder, Ark Metrica & TerraChange Solar

Group Website: https://www.physics.ox.ac.uk/research/group/advanced-functional-materials-and-devices-afmd-group

### List of Abstracts for Oral Presentations

#### **Oral Presentation Session 1**

#### 15:15 - 15:25 Dr. Theodore Hobson (Department of Materials)

#### Solar Cell Design for a Multi-Terawatt Future

Solar photovoltaics are currently experiencing exponential growth globally, with a 4x expansion in capacity projected by 2030, and 40x projected by 2040. Maintaining this astonishing trajectory will require continuous improvement in two areas: -Solar cell designs must enable ever greater power-conversion efficiencies -The materials used in their manufacture must be of an abundance consistent with global solar installations on the multi-10x terawatts scale. I will present ongoing collaborative work between the Departments of Materials and Physics to address both challenges: -I will discuss our development of two-junction 'tandem' solar cells to enable major efficiency gains over current technologies. -I will also cover how we are working to reduce the proportion of indium, a valuable but globally scarce element, in our high-efficiency cell designs. As such, these studies will support the development of higher performance solar cells which can be produced on the scale necessary to eliminate carbon emissions.

#### 15:25 - 15:35 Dr. Yige Sun (Department of Materials)

#### Mapping Li Concentration Gradients across Battery Cathodes

Lithium-ion batteries (LIBs) are essential for low-carbon energy storage, but optimizing electrode design remains challenging due to complex ion transport dynamics. Thick electrodes enhance volumetric capacity but suffer from Li-ion concentration gradients, leading to uneven active material utilization and degradation. Traditional techniques like energy dispersive X-ray spectroscopy (EDS) cannot resolve Li distributions effectively. This study develops a methodology using secondary ion mass spectrometry (SIMS) to visualize Li-ion concentration gradients in LIB cathodes, integrating SIMS with EDS and plasma field ion microscopy (P-FIB) for 3D analysis. Applied to LiFePO<sub>4</sub> (LFP) and LiMn<sub>2</sub>O<sub>4</sub> (LMO) electrodes of varying thickness and charge states, this approach captures cross-sectional Li distributions with high spatial resolution. By correlating EDS and SIMS maps, it accounts for factors affecting <sup>7</sup>Li<sup>+</sup> intensity, revealing fine-scale variations linked to microstructural features. This method provides insights into electrode performance and degradation mechanisms, informing future LIB design improvements.

#### 15:35 - 15:45 Robin Nicholson (Oxford School of Global and Area Studies)

#### Japan's Push for Hydrogen: Will it Work (this time)?

Japan wants to create a 'hydrogen society', where hydrogen is used in all sectors of the economy. With hydrogen, Japan aims to increase its domestic energy security and self-sufficiency, boost green industrial growth with fuel-cell vehicles and hydrogen-based technology for export overseas, and meet global carbon emissions reductions targets by 2050. Japan also intends to lead in establishing global regulations governing international hydrogen supply chains and technology (Naikakufu 2023). Hydrogen is not new for Japan, having existed in various iterations through cycles of hype and crash since 1972. In this latest iteration, since 2014, the government has been promoting its hydrogen strategy using green industrial policy tools such as long-term target setting and financing. Yet, as many countries and companies are now reducing or abandoning their hydrogen production targets and strategies, Japan is persisting. Will it ultimately succeed this time?

#### 15:45 - 15:55 <u>Matthew Williams (Department of Chemistry)</u>

### Ultra-high surface area layered double hydroxide-based nanomaterials for sustainable chemistry

Hydrogen is a promising energy vector, with a gravimetric energy density three times higher than conventional hydrocarbon fuels. However, over 95% of hydrogen production relies on fossil fuels, generating carbon emissions. Electrochemical hydrogen production from water offers a low-carbon alternative, but the energy required to drive the oxygen evolution reaction (OER) is a challenge. The process requires overcoming slow reaction kinetics and relies on expensive heavy-metal catalysts like ruthenium and iridium. Designing highly-active electrocatalysts from Earth-abundant transition metals (Fe, Co, and Ni) offers a promising, scalable, low-cost alternative. Related layered double

hydroxides (LDHs) exhibit excellent OER activity, have inexpensive syntheses, and are highly tuneable with a variety of applications. Development of LDH electrocatalysts focuses on improving catalytic efficiency by enhancing intrinsic activity or increasing exposed active sites. This research focuses on the structural engineering of LDHs to synthesise ultra-high surface area nanosheets capable of enhanced electrocatalytic efficiency for hydrogen production.

#### 15:55 - 16:05 Dr. Junzhi Ye (Department of Chemistry)

### Extending the defect tolerance of halide perovskite nanocrystals to hot carrier cooling dynamics

Defect tolerance is a critical enabling factor for efficient lead-halide perovskite materials, but the current understanding is primarily on band-edge (cold) carriers, with significant debate over whether hot carriers can also exhibit defect tolerance. Here, this important gap in the field is addressed by investigating how intentionally introduced traps affect hot carrier relaxation in CsPbX<sub>3</sub> nanocrystals (X = Br, I, or mixture). Using femtosecond interband and intraband spectroscopy, along with energy-dependent photoluminescence measurements and kinetic modelling, it is found that hot carriers are not universally defect tolerant in CsPbX<sub>3</sub> but are strongly correlated to the defect tolerance of cold carriers, requiring shallow traps to be present (as in CsPbI<sub>3</sub>). It is found that hot carrier sare directly captured by traps, instead of going through an intermediate cold carrier, and deeper traps cause faster hot carrier cooling, reducing the effects of the hot phonon bottleneck and Auger reheating. This work provides important insights into how defects influence hot carriers, which will be important for designing materials for hot carrier solar cells, multiexciton generation, and optical gain media.

#### **Oral Presentation Session 2**

#### 17.15 - 17:25 Shaoni Kar (Department of Physics)

#### Evaporated inorganic perovskites for light emission

Perovskite semiconductors, among many other applications, are outstanding candidates for light emission. Enabling solvent-free scale up and uniformity across large areas, evaporated perovskites have, in the recent years, been reported for their superior performance in displays and light emitting diodes (LEDs). However, in contrast to their more ubiquitous solution-processed counterparts, they suffer from lower photoluminescence and electroluminescence quantum yields (PLQE/EQE) due to higher defect densities, difficulty in regulating crystallisation and morphology etc. In Oxford's cluster deposition facility, we have developed operational LEDs emitting across the visible (red, green, blue) and infrared ranges based on thermally evaporated perovskites. In a field already limited by several fundamental challenges, we currently hold the record for the world's most efficient (3.5%) pure-red LEDs. In this work, we investigate the morphology and corresponding photophysical properties of these films, their electrical characteristics as well as their device performance.

#### 17:25 - 17:35 Claire Torina Coulthard (Department of Chemistry)

#### Novel materials for CO<sub>2</sub> conversion: Challenges and opportunities

My research focuses on the development of materials for the conversion of carbon dioxide into high-value products, such as methanol and diesel alternatives. In this presentation, I will provide an overview of the current advancements in carbon dioxide utilisation, as well as mentioning the obstacles associated with implementation and scale-up. Additionally, I will share findings from my own work designing multifunctional materials for efficient carbon dioxide conversion. Here, we have designed hybrid materials for the thermocatalytic conversion of  $CO_2$  to methanol and dimethyl ether.

#### Hybrid processing of perovskite thin films for terawatt-scale photovoltaics

Solar panels incorporating perovskite materials in tandem with silicon have claimed centre stage in ensuring that the levelized cost of electricity of solar continues to fall by enabling more power generation per unit area than silicon-only photovoltaics. Two barriers to widespread adoption of perovskite-silicon tandem panels are the availability of wide-area processing methods for perovskite thin films and the need to avoid hazardous solvents in processing. A novel film deposition technique consisting of thermal evaporation of a lead halide precursor, followed by spin coating of organic salts dissolved in environmentally benign solvents is presented as a solution. The resulting high-quality, phase-pure formamidinium lead iodide film crystallises from a low-dimensional intermediate, demonstrating the promise of this approach for processing wide-bandgap absorber layers in perovskite/silicon tandems. This opens an additional pathway to utility-scale perovskite integration into the grid.

#### 17:45 - 17:55 Xiaohang Cai (Department of Materials)

#### Advancing Flexible Thermoelectric Generators for Wearable Energy Harvesting

Flexible wearable electronics are rapidly evolving, driving demand for compact and efficient energy solutions. Thin-film thermoelectric generators (TEGs) provide a promising complementary power source by converting body heat into electricity, reducing reliance on frequent recharging. However, their integration into flexible systems is often limited by material brittleness and fabrication challenges. This research advances scalable, high-performance TEG architectures through three key strategies: (1) investigating soft-brittle interface degradation under mechanical stress to enhance durability, (2) engineering temperature gradients using deformable thin-film aerogels to maintain efficiency in thin-film devices, and (3) implementing a multilayer design—stacking thousands of ultrathin TE layers to achieve high power density while preserving flexibility in practical applications. By combining material and design innovations with scalable fabrication, this work takes a crucial step toward making thermoelectric energy harvesting a viable solution for real-world flexible electronics.

#### 17:55 - 18:05 Haozhe Zhang (Department of Chemistry)

#### Tuning Layered Perovskite for Efficient Photocatalytic NH<sub>3</sub> Decomposition

Photocatalytic decomposition of NH<sub>3</sub> with reducing heat is essential for decreasing H<sub>2</sub> production costs. However, efficient photocatalysts for NH<sub>3</sub> decomposition are scarce, hindering the further application of this technology. Herein, we present a hydrazine-intercalated layered perovskite,  $(N_2H_4)_{0.5}$ PrNb<sub>2</sub>O<sub>7</sub>H, which exhibits the highest NH<sub>3</sub> decomposition rate compared with all photocatalysts reported in literature. This study is also the first to report this unique property of perovskite oxides, wherein N<sub>2</sub>H<sub>4</sub> molecules can be stabilised within the interlayer gallery. Our extensive characterisations successfully determined the precise occupancy and position of N<sub>2</sub>H<sub>4</sub> molecules in the perovskite structure, elucidating the formation process of N<sub>2</sub>H<sub>4</sub> within the interlayer space. Moreover, Ru<sup>2+</sup> doping into the perovskite matrix significantly enhanced the photocatalytic performance. With the progressive increase of temperature during photocatalysis, the H<sub>2</sub> evolution rate could reach to ~2.3 mmol/gh at 200 °C, highlighting the synergistic effect of thermal and photo contributions to NH<sub>3</sub> decomposition.

#### 18:05 - 18:15 Lorenzo Catini (Department of Chemistry)

## Exploring photophysical mechanisms in organic solar cells through electrically detected magnetic resonance

Organic Solar Cells (OSCs) support the renewable energy transition by enabling new applications such as buildingintegrated photovoltaics, indoor photovoltaics and wearable technologies, thanks to the ability to tune the flexibility, colour and transparency of devices with organic molecules as the active layer. In recent years, a new series of organic acceptor molecules (known as the Y-series) has enabled a significant increase in power conversion efficiency, now exceeding 20%. However, the details of the photophysical processes underlying device function for solar cells based on these new acceptor molecules are not yet fully understood. We use Electrically Detected Magnetic Resonance (EDMR) spectroscopy to study charge carrier dynamics in fully working, miniaturized OSCs by exploiting the electron spin associated with each charge as a probe. An in-depth understanding of fundamental mechanisms and of correlations between molecular structure and device performance will be key to aid the design of new and more efficient molecules.

### List of Abstracts for Flash Talks

#### 16:45 - 16:48 George Carew-Jones (Smith School)

#### Understanding routes to energy project bankability in Zambia

Bankability is central to understanding how Zambia's ambitious energy sector expansion plans can be achieved. With private sector finance being a necessary ingredient for rapid infrastructure delivery, this research explores what key energy sector stakeholders in Zambia think are the most promising routes to achieving improved energy project bankability. We find that progress has been made in core areas, with market liberalisation reforms and improved creditworthiness for the state-owned energy utility (ZESCO) setting the conditions for Zambia to access new pools of concessional and commercial finance. To consolidate progress, this policy brief points to four concrete priority areas to reduce investor risk: (i) liberalised offtake agreements, (ii) increased and differential tariffs, (iii) the creation of a 'one-stop shop' for permitting, and (iv) diversified access for investors and novel instruments. These steps are crucial to derisking projects and raising revenues, thereby lowering the cost of capital available to energy project developers.

#### 16:48 - 16:51 Kanksshi agarwal (Blavatnik School of Government)

#### An analysis of relevant political narratives emerging in global south

#### 16:51 - 16:54 Karan Mukhi (Department of Computer Science)

#### Aggregation of Flexibility in Populations of Distributed Energy Resources

As renewable energy adoption grows, power systems require greater flexibility to balance supply and demand. My work focuses on developing a mathematical framework to accurately characterize and optimize the flexibility in populations distributed energy resources (DERs), particularly electric vehicles (EVs). Using geometric representations called generalized polymatroids, we provide an exact method to aggregate flexibility across populations of devices. Our approach enables power system operators and aggregators to efficiently manage demand-side resources and participate in flexibility markets. Additionally, we extend this framework to account for uncertainty in EV charging behavior, using distributional robust optimization methods to ensure reliable operation. My work offers a scalable solution for integrating DERs into the grid and mitigating the intermittency and uncertainty of renewable generation.

#### 16:54 - 16:57 Dr. Phil Grunewald (Department of Engineering Science)

#### Observing and changing household energy use with better data, information and messages

We generate and use energy to meet our energy service needs, such as staying warm, moving about and exchanging information. How and when we meet these needs is still poorly understood. We gather detailed in-home data (energy and other) to learn more, and action effective changes to energy demand, while maintaining or improving our energy services.

#### 16:57 - 17:00 Marcel Seger (Environmental Change Institute)

## Firm level optimisation strategies for sustainable and cost-effective electric vehicle workplace charging

Expanding electric vehicle (EV) charging infrastructure is essential for transi- tioning to an electrified mobility system. With rising EV adoption rates, firms face increasing regulatory pressure to build up workplace charging facilities for their employees. However, the impact of EV charging loads on businesses' specific electricity consumption profiles remains largely unknown. Our study addresses this challenge by presenting a mathematical optimisation model, available via an open-source web application, that empowers business executives to manage energy consumption effectively, enabling them to assess peak loads, charging costs, and carbon emissions specific to their power profiles and employee needs. Using real-world data from a global car manufacturer in South East England, UK, we demonstrate that smart charging strategies can reduce peak loads by 28% and decrease charging costs and emissions by 9% compared to convenience charging. Our methodology is widely applicable across industries and geographies, offering data-driven insights for planning EV workplace charging infrastructure.

## The Role of Building Energy Simulation in Achieving Net-Zero Operating Emissions in the UK Non-Domestic Building Sector

90% of existing buildings will still be standing in 2050, year by which the Paris Agreement requires all sectors to be netzero. Accelerating the decarbonisation of the building sector is critical. My research focuses on the use of Building Energy Simulation (BES) tools to evaluate decarbonisation strategies through virtual modelling of energy conservation measures. Using the University of Oxford buildings as case studies, I examine how BES accuracy balances with complexity and data requirements. I develop methods to make BES more accessible and user-friendly, while investigating how modelling simplifications affect its reliability. This research also explores BES applications for climate adaptation and grid integration, aiming to create a framework that promotes wider BES adoption for energy assessment and policy development.