KING'S College LONDON

Tackling Future Net Zero Challenges

Net Zero Centre annual event

Agenda

09:30 - 10:00	Registration
10:00 – 10:05	Opening remarks from Professor Barbara Shollock, Professor Anatoly Zayats & Professor Raúl Rosales Araque
10:05 – 10:10	'*New materials towards obtaining net zero'* presented by Professor Mark Green
10:10 – 10:20	'*The synthesis, reactivity and computational analysis of low oxidation state Group 13 complexes'* presented by Michelangelo Tritto
10:20 – 10:30	'*The EV transition: the impact of the EU battery regulation on critical material supply, recycling and battery costs*' presented by Malene Fumany
10:30 – 10:40	'*Vapour deposited perovskites for high performance multi-junction solar cells'* presented by Hallie Echelman
10:40 – 10:50	Break
10:50 – 10:55	'*A system's engineering framework for sustainable transport*' presented by Professor Rym M'Hallah
10:55 – 11:05	'*Stochastic modelling of electricity demand on multiple time scales*' presented by Zining Yuan
11:05 – 11:15	*'Data-driven optimization for shared micromobility logistics*' presented by Haoxiang Wang
11:15 – 11:25	'*Living systems thinking*' presented by Dr Emma Fromberg
11:25 – 11:35	Break
11:35 – 11:40	'*Innovations for sustainable manufacturing*' presented by Dr Alex Brogan
11:40 – 11:50	'*Biocatalytic recycling of polyurethane with stabilized Proteinase K in ionic liquids*' presented by Annika Dennis
11:50 – 12:00	'*Data-driven prediction of global warming potential for sustainable manufacturing*' presented by Jaewook Lee
12:00 – 12:10	'*Fabrication of nanomaterials for net zero*' presented by Henry Cossey
12:10 – 12:15	Break
12:15 – 12:30	'*Carbon markets: AI-powered simulations for market analysis & design*' presented by Professor Carmine Ventre
12:30 – 12:45	**'***Product-mix auctions for integrating greenhouse gas removals into the UK ETS*' presented by Dr Edwin Lock
12:45 – 12:55	'*Agent-based analysis of green disclosure policies and their market-wide impact on firm behaviour*' presented by Lingxiao Zhao
12:55 – 13:00	Closing remarks from Professor Frans Berkhout
13:00 – 14:00	Lunch & Networking

Abstracts

New materials towards obtaining net zero

Professor Mark Green

Achieving net zero emissions requires a fundamental transformation in how materials are designed, produced and reused. This presentation outlines the critical role of materials innovation in decarbonisation—from reducing the carbon footprint of high-emission sectors such as steel and cement to enabling next-generation technologies including photovoltaics, thermoelectrics and low-loss electronics. Drawing on interdisciplinary strengths across Physics, Chemistry and Engineering at King's, we highlight how integrated approaches to materials discovery, circularity and lifecycle design can accelerate the transition to a sustainable, net zero future.

The synthesis, reactivity and computational analysis of low oxidation state Group 13 complexes

Michelangelo Tritto

Transition metals represent the gold standard when it comes to chemical catalysis. In recent years however, questions have been raised regarding their long-term use, especially when considering the scarcity of many frequently employed catalytic metals (Pt,Pd, Rh, Ir) and the unethical practices commonly associated with their extraction. Group 13 elements (B, Al, Ga, In) in their lower (electron rich) oxidation states, have shown great promise in recreating aspects of transition metal reactivity, whilst remaining generally free of these burdens.

Michelangelo's PhD research focuses on tuning these elements (in particular aluminium and indium) to mimic useful 'transition metal-like' reactivity. Whilst conceptually attainable, bonding in main group compounds can often be quite complex, commonly breaking conventional classification 'rules' and making their reactivity hard to predict or control.

The EV transition: the impact of the EU battery regulation on critical material supply, recycling and battery costs

Malene Fumany

Lithium-ion batteries (LIBs) are central to current international Net Zero strategies. However, regulations and geopolitics have increased the risk of bottlenecks in the supply of critical battery materials that could endanger the global push to Net Zero. The urgency of the situation led to the introduction of policies aimed at establishing local battery ecosystems including the recycling of end-of-life LIBs. However, the impact of these policies on material dependencies and battery economics is not well understood. This study introduces a policy-economic framework that is used to assess the potential evolution of the LIB recycling sector in response to policy changes supported by findings from an industry-led survey. The European Union Battery Regulation is analysed to understand the impact of its mandated minimum recycled content on materials and battery costs for a range of different battery chemistries. This study provides new evidence on how international policies and legislations may impact the future of the battery sector

Vapour deposited perovskites for high performance multi-junction solar cells

Hallie Echelman

Silicon-based photovoltaics have long dominated the solar energy market due to their technological maturity accredited to decades of dedicated research. However, single-junction silicon devices are intrinsically constrained by the Shockley–Queisser limit and have approached their practical efficiency ceiling of ~27%. Metal-halide perovskites have emerged as a promising class of materials to overcome this limitation due to various remarkable optoelectronic properties, including a tuneable bandgap through compositional substitutions which reduces thermalization losses and allows for tailored spectral absorption [1]. By enabling absorption across defined regions of the solar spectrum, perovskites are especially well-suited for integration into multijunction architectures where triple-junction efficiencies exceeding 50% are theoretically achievable. While most perovskite research has focused on solution-based synthesis techniques, thermal evaporation offers significant advantages such as nanometre-scale thickness control, high reproducibility, and compatibility with large-area deposition [2]. Moreover, silicon manufacturing is highly energy intensive due to extreme purity and high-temperature processing requirements, whereas perovskites can be fabricated using lower-energy and less wasteful routes, allowing for more sustainable manufacturing. In addition, their ultrathin and lightweight nature enables advancements in flexible and building-integrated photovoltaics, expanding the implementation landscape for solar energy [1]. By leveraging these advantages, this work demonstrates the development of a fully evaporated 2.0eV wide-bandgap inorganic perovskite semiconductor as a top absorber in triple-junction devices, establishing a promising route toward high-efficiency, sustainable photovoltaics for a net-zero future.

References

[1] Blakesley, J. C., Bonilla, R. S., Freitag, M., Ganose, A. M., Gasparini, N., Kaienburg, P., Koutsourakis, G., Major, J. D., Nelson, J., Noel, N. K., Roose, B., Yun, J. S., Aliwell, S., Altermatt, P. P., Ameri, T., Andrei, V., Armin, A., Bagnis, D., Baker, J., … Hoye, R. L. Z. (2024). *Journal of Physics: Energy*, *6*(4), 041501.

[2]Abzieher, T., Moore, D. T., Roß, M., Albrecht, S., Silvia, J., Tan, H., Jeangros, Q., Ballif, C., Hoerantner, M. T., Kim, B.-S., Bolink, H. J., Pistor, P., Goldschmidt, J. C., Chiang, Y.-H., Stranks, S. D., Borchert, J., McGehee, M. D., Morales-Masis, M., Patel, J. B., … Paetzold, U. W. (2024). *Energy & Environmental Science*, *17*(5), 1645–1663.

A system's engineering framework for sustainable transport

Professor Rym M'Hallah

This four-step framework offers a systemic approach that is efficient, effective, scalable, and explainable while nudging behaviour changes and adoption, offering a cost-effective service, and balancing supply and demand. First, the framework builds a rich understanding of real-world challenges through an exchange of users' perspectives -during workshops for industry, government, and charities, and both surveys and focus groups for users-. Second, it integrates behaviour insights into mathematically based,

implementable, sustainable, cost-effective, solutions for the revealed real-world challenges (e.g., green transport and transportation, health care, manufacturing). For this purpose, it explores Systems Engineering to conceive, create, develop, and apply multi-criteria optimization for real-life processes that bring a high degree of complexity, resorting to discrete-event and agent-based simulation and system dynamics to validate the outcomes. Third, it transforms these solutions into a Human centred information-driven decision making for industry, government, and service in socially and economically critical sectors, and Strategic foresight (e.g., for mobility stakeholders in the UK). Fourth, it uses the research outcomes to inform policy agendas and identify policy gaps.

Stochastic modelling of electricity demand on multiple time scales

Zining Yuan

Developing a stochastic model for half-hourly electricity demand in Great Britain in the mid-term: The model captures annual, weekly and daily seasonal patterns as well as temperature dependencies through semi-parametric additive models. The model allows for the incorporation of expert views and other information that may not be contained in historical data. The model is easy to implement and computationally fast, which makes it useful for long-term electricity price simulations and risk management. The model was developed in collaboration with the UK government entity, Low Carbon Contracts Company.

Data-driven optimization for shared micromobility logistics

Haoxiang Wang

As cities worldwide pursue net-zero emissions by 2050, urban transportation systems are undergoing a major shift toward shared, on-demand services that must operate reliably at city scale. Shared micromobility has emerged as a flexible, low-carbon alternative for short-distance travel. However, asymmetric travel patterns cause inventory imbalance, and users frequently encounter stations with no vehicles available for pickup or no docking capacity for returns. Such unfulfilled demand adversely affects user retention and system adoption. Maintaining service quality therefore requires effective rebalancing, the redistribution of vehicles among stations. Rebalancing is challenging due to the large scale of networks, the inherent trade-off between operating cost and service level, and the presence of demand uncertainty. This talk presents data-driven optimization tools that help micromobility operators keep vehicles where riders need them, demonstrated using real operations data from London's Santander Cycles.

Living systems thinking

Dr Emma Fromberg

Drawing on her research in sustainable business, Dr Emma Fromberg uses metaphors from nature to understand our economic systems as "living": non-linear, dynamic and resistant to being fully captured by dominant Western logic.

Innovations for sustainable manufacturing

Dr Alex Brogan

The manufacture of chemicals, fuels, and materials has a significant impact on global emissions. It is therefore imperative that we develop new technologies and processes to simultaneous make manufacturing more efficient and to move away from oil-based resources. This talk will briefly provide the backdrop to introduce the session on sustainable manufacturing with talks that cut across the full spectrum of what is required to realise net zero in this space.

Biocatalytic recycling of polyurethane with stabilized Proteinase K in ionic liquids

Annika Dennis

With the high stability and durability of commercial plastics, there is a need for sustainable plastic recycling methods, to overcome the current limitations of both high energy requirements and low-quality products. Enzymes are promising catalysts for plastic depolymerization due to their high efficiency, mild reaction conditions, and low environmental impact. However, enzymes are unstable in conditions required for recycling, limiting the window of usability for industrial processing. Chemical modification of enzymes can enhance thermal stability and structure retention by coupling polymer surfactants to the enzyme, a technique previously used for biomass processing in ionic liquids.1 In this study, polymer degradation via enzyme-catalyzed hydrolysis in ionic liquid was accomplished using chemically modified hydrolases, including cutinase and proteinase K. Retained structure and thermal stability of modified enzymes was established using circular dichroism (CD), dynamic light scattering (DLS), and enzyme activity assays. The stability of the modified hydrolases in ionic liquids was studied using synchrotron radiation circular dichroism (SRCD). Furthermore, differential scanning calorimetry (DSC), showed that ionic liquids reduced polymer crystallinity, lowering the barrier for enzymatic degradation reactions. The chemically modified hydrolase degradation activity showed that modified cutinase stabilized in [emim][EtSO4] improved PET degradation from 1.55% to 4.50% after heating for 24 hours at 120°C. Further, proteinase K stabilized in [emim][OAc] exhibited activity towards polyurethane, with 57.70% degradation after heating for 24 hours at 60°C. This study demonstrates the potential of employing chemically modified enzymes in ionic liquids for effective plastic recycling.

Data-driven prediction of global warming potential for sustainable manufacturing

Jaewook Lee

Accurate yet interpretable prediction of Global Warming Potential (GWP) is essential for the sustainable design of molecules, materials, and chemical processes. In this work, I present an AI-based GWP prediction framework that integrates molecular descriptors and process-level information to support early-stage environmental screening. A deep neural network model achieves high predictive accuracy by jointly leveraging molecular features and process context, while explainable AI analysis highlights the importance of process-related information. To address the need for transparency, a complementary white-box

model based on Kolmogorov–Arnold Networks is introduced, providing explicit mathematical relationships between inputs and GWP. Together, these approaches demonstrate how data-driven models can balance accuracy and interpretability, offering practical support for sustainable manufacturing and early-stage assessment of compounds relevant to carbon management and CCUS applications.

Fabrication of nanomaterials for net zero

Henry Cossey

Moving from bulk materials down to the nanoscale, a number of interesting effects can present themselves in the way light interacts with matter. This talk will cover some of the ways in which we can fabricate materials that respond strongly with light, giving us another way to utilise an abundant source of energy.

Carbon markets: AI-powered simulations for market analysis & design

Professor Carmine Ventre

This talk explores how AI-powered, agent-based simulations and empirical game-theoretic analysis can be used to analyse and design carbon markets. Using recent work calibrated to real emissions trading schemes, we will see how these tools help fine-tune market rules to reduce emissions without sacrificing economic productivity.

Product-mix auctions for integrating greenhouse gas removals into the UK ETS

Dr Edwin Lock

The UK Emissions Trading Scheme (UK ETS) is a cap and trade covering the heavy industry, power, and aviation sectors. Businesses acquire UK emissions allowances (which they can surrender to cover their emissions) through free allocations, and through auctions of carbon allowances. In 2023, the UK confirmed that allowances from greenhouse gas removals (GGRs) should be included in the UK ETS by 2029.

We proposed to the UK Department for Energy Security and Net Zero that they use a Product-Mix Auction to integrate GGRs into the UK ETS. The PMA was originally designed for, and is still used regularly by, the Bank of England to provide liquidity to financial institutions. The auction treats UKAs and GGRs as differentiated goods, and bidders can bid on either UKAs, or GGRs, or place bids jointly on both to receive the option they prefer at market prices. The PMA would be more efficient than running separate auctions for UKAs and GGRs.

Agent-based analysis of green disclosure policies and their market-wide impact on firm behaviour

Lingxiao Zhao

Green disclosure policies are designed to help firms communicate their environmentally friendly practices to investors. While most research has focused on the effects of these policies at the individual firm level, their influence within a system of multiple firms remains largely unexamined. To address this gap, we develop an agent-based model to simulate market dynamics among firms with varying levels of environmental performance and strategic responses. Using Empirical Game-Theoretic Analysis, we investigate how the costs associated with becoming greener and investors' valuation of these efforts shape equilibrium outcomes and the prevalence of green firms in the market. Our findings reveal that changes in the cost of green upgrades significantly influence firms' strategic choices and alter the equilibrium behaviour of the other firms. Additionally, we analyse the effects of different green disclosure policies and find that under more relaxed policies, firms are more willing to incur into higher upgrade costs. Furthermore, we propose a two-stage disclosure policy that incentivizes all types of firms to enhance their green practices, thereby promoting the broader adoption of sustainable energy solutions across the market.

Speaker biographies

Barbara Shollock is the Founder and Director of Net Zero Centre and Professor of Engineering at King's College London. She was Head of Department between 2019–2024, when the Department of Engineering was re-founded at King's College London. Her research on focuses on phase transformations from the nano- to micro-scale has provided fundamental theoretical and experimental insight into the understanding, development, and performance enhancement of a range of engineering materials and the development of new materials. Her research outputs have played key roles in advancing important aspects of the UK engineering industry.

Anatoly Zayats is the head of the Photonics & Nanotechnology Group at King's College London. He is a Co-Director of the London Centre for Nanotechnology, the Net Zero Centre and the London Institute for Advanced Light Technologies. He is a founding co-editor-in-chief of Advanced Photonics. He is a holder of the Royal Society Wolfson Research Merit Award, a Fellow of the Institute of Physics, the Optical Society of America, SPIE and the Royal Society of Chemistry and an elected Member of Academia Europaea.

Raúl Rosales Araque is a Professor of Practice in Net Zero Asset Management within the Department of Engineering at King's College London. He also works as a Senior Advisor for Orchard Global Asset Management LLP, an Alternative Credit Investment Fund in London. His background in the financial industry spans 30 years, most recently at the European Bank for Reconstruction and Development (EBRD) as Senior Banker for Energy and previously at BBVA as Global Head of Multilateral Banks (MDBs). He is a Doctor in Civil Engineering, specialising in sustainable infrastructure and energy. He leads research on carbon markets and capital mobilisation, connecting engineering solutions with policy and finance to accelerate industrial decarbonisation.

Mark Green obtained his chemistry degree from Manchester Metropolitan University in 1995, followed by a PhD in quantum dot synthesis from Imperial College in 1998. This was followed by post-doctoral positions at Imperial and Oxford. In 2000, he was then an early employee of Oxonica, a spin-out company from The Department of Engineering at the University of Oxford until 2004, when he was appointed as a lecturer in nano-biophotonics in the Physics Department at King's College London where he was promoted to Professor of Nanotechnology in 2014. His work cover organometallic, inorganic and organic materials chemistry with applications in biology.

Michelangelo Tritto is a 3rd year PhD student funded by the KCL Net Zero centre. He previously completed his MSci project at KCL in the Bakewell group (2023), making main-group metal hydrides, exploring their reductive chemistry and analysing them computationally. He was awarded the King's Layton Science Research Award for this project.

Malene Fumany is undertaking her PhD under the supervision of Dr Laura Lander at King's College London in the Green Energy Materials Lab. Malene has a Bachelor's in chemical engineering from the University of Bradford and a Master's in Petroleum Engineering from Imperial College London. Malene has industry experience in battery research and recycling from working at Nissan as a Battery Research Engineer Contractor before moving to WMG, in Warwick, as a project engineer in hydrometallurgical recovery. Her research focuses on recycling of lithium-ion and next-generation batteries, where she conducts techno-economic and business analyses as well as optimises battery recycling processes.

Hallie Echelman is a PhD candidate in Physics at King's College London, working under the supervision of Dr. Jay Patel in the Functional Materials and Devices Laboratory. Her doctoral research focuses on advancing multi-junction perovskite solar cells through vapor deposition techniques, with the aim of enabling more efficient and sustainable next-generation photovoltaic devices. Prior to her PhD, Hallie earned a Bachelor's degree in physics from Skidmore College (New York, USA), followed by a Master's degree in physics with a specialization in Energy and Sustainability through a joint program at the University of Amsterdam and Vrije Universiteit Amsterdam. She has also held several full-time professional roles, including R&D Laser Engineer in New York, at a clean-technology startup in Tel Aviv, Israel, and as an IT Energy Consultant in the Netherlands.

Professor Rym M'Hallah is Chair in Systems Engineering at King's College London and holds a BS, MS, and PhD in Industrial and Systems Engineering, all from the Pennsylvania State University. Her research advances systems thinking, sustainability and optimisation, with work spanning shared services, resource management and supply-chain resilience. She leads a £1.2M EPSRC project on behavioural and operational approaches to improve resource use and serves on editorial boards of leading Operations Research journals. Her current focus includes sustainable urban mobility and healthcare systems engineering, alongside collaborations with industry, charities and government.

Zining (Pearl) Yuan is a third-year PhD researcher in climate finance whose work focuses on the pricing and resilience of the energy and financial markets to climate shocks.

Haoxiang Wang is a 4th-year PhD candidate in Computer Science at King's College London. His interests include sequential optimization and learning under uncertainty, with applications to sustainable supply chain management and revenue management.

Emma Fromberg is a Research Fellow affiliated with the Centre for Sustainable Business at King's Business School, with extensive experience in sustainable business and sustainable value chains. Trained as an Industrial Design Engineer and Strategic Product Designer, Emma is interested in how business-led activities can contribute to system-level change to support the transition to a more regenerative, accessible and abundant economy. Her research focuses on drawing lessons from nature and ecology to inform how one could reimagine the economy.

Alex Brogan is a Senior Lecturer in the Department of Chemistry at King's College London, having started his independent career there in 2019. Alex obtained both his MSci and PhD from the University of Bristol and did his postdoc at Imperial College London where he also spent time as a Visiting Scientist at the Massachusetts Institute of Technology. The focus of his research is to develop new biotechnologies to make biological systems more compatible with synthetic systems. The purpose of which is so that we can fully exploit nature's toolkit to make our own industry more sustainable and more environmentally friendly, whilst simultaneously helping us move from an oil-based economy to a bio-based economy.

Annika Dennis is a third-year PhD student in the Department of Chemistry at King's College London, where her research focuses on developing sustainable approaches to plastic recycling. Her work explores how enzymes can be stabilized in ionic liquids to selectively depolymerize challenging plastics such as polyurethane under mild conditions. Motivated by the potential for chemistry to address real environmental problems, Annika is particularly interested in using creative, biologically inspired strategies to enable circular solutions for materials that are currently considered unrecyclable.

Jaewook Lee is a PhD Researcher in the Department of Engineering at King's College London, supervised by Dr Miao Guo and Prof Chris Lorenz. His research focuses on AI-enabled environmental assessment and sustainable process design, with current work on data-driven prediction of environmental impacts in chemical manufacturing. He is particularly interested in applying advanced computational methods, including molecular simulation, machine learning, and large language models, to challenges in Process Systems Engineering and net-zero technologies.

Henry (Harry) Cossey is a PhD student within the Photonics & Nanotechnology group at King's College London, UK. His research focuses on the fabrication and characterisation of photonic materials and nanostructures, under the supervision of Professor Anatoly Zayats.

Carmine Ventre is a Professor of Computer Science and Chair in Computational Finance in the Department of Informatics, King's College London. He gained a Laurea degree and a PhD in Computer Science, both from Università di Salerno. He subsequently worked at the University of Liverpool, Teesside University and the University of Essex before joining King's in September 2019, to lead the Finance research hub in the Department of Informatics. He has also been the director of the King's Institute for AI and the Head of the Department of Informatics. Professor Ventre's research interests include algorithmic game theory, microeconomics and the internet, AI for algorithmic trading and finance and cryptography and security.

Edwin Lock is a Lecturer in Computer Science at King's College London. His work focuses on computational questions arising in auction and market design. In his research, he aims to combine research at the core of theoretical computer science with applications to problems of key societal importance. Before taking up his position at King's, he was a postdoctoral researcher at Oxford University. He is also an Associate Member of Nuffield College, Oxford. For more information, see www.edwinlock.com.

Lingxiao Zhao is a Research Software Engineer at IOG (Input Output Group), working on large-scale simulation engines for decentralised governance modelling. Before this role, he completed a PhD in Computer Science at King's College London, focused on strategic behaviour and equilibrium in financial systems using agent-based and game-theoretic methods. Dr. Zhao's research interests include tokenomics, algorithmic game theory, multi-agent systems, agent-based modelling, and ESG modelling, with publications in venues such as AAMAS, ICAIF, and PRIMA.

Frans Berkhout is Professor of Environment, Society and Climate in the Department of Geography at King's College London. He also serves as Assistant Principal (King's Climate & Sustainability) and Assistant Principal (Academic Freedom and Freedom of Expression) at King's. Over the past 25 years, his research has been concerned with science, technology, policy and the environment, with a focus on sustainable innovation and climate change.