UK Symposium on Materials for Sustainability

1 July 2025

Keele University, Staffordshire, UK

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Programme: Tuesday 1 July 2025

8:50 AM - 9:20 AM	Registration and Refreshments
9:20 AM - 9:30 AM	Welcome Talk
9:30 AM - 10:00 AM	**Invited Talk: Prof. Amalia Patane** Atomically Thin Semiconductors for Science and Technology
10:00 AM - 10:30 AM	**Invited Talk: Dr. Abhishek Misra** Room Temperature Dipolar Excitons in van der Waals Heterostructures
10:30 AM - 11:00 AM	**Invited Talk: Dr. Yan Wang** Clean interfaces on 2D semiconductors
11:00 AM - 11:15 AM	Morning Break
11:15 AM - 12:15 PM	**Oral Contributions** **11:15 AM - 11:30 AM Jason Stafford** Sustainable liquid phase exfoliation processes for 2D materials using predictive models and feedstock re-use **11:30 AM - 11:45 AM Geeta Sharma** Tailoring optical and thermal properties in rare-earth doped MoS_2 for device applications **11:45 AM - 12:00 PM Deepa Bhatt** Effect of Te substitution and copper vacancies on the thermoelectric performance of BiCuSeO **12:00 PM - 12:15 PM Melanie Randall-Evans** Assessing the discharge-recharge mechanism of monovalent cation-directed hausmannite Mn_3O_4 cathodes in aqueous Zn-ion batteries
12:15 PM - 12:45 PM	**Invited Talk: Dr. Zeeshan Ali** Development of Nucleophilic Metal-Seeded Anodes for Enhanced Sodium Metal Batteries
12:45 PM - 1:10 PM	Poster Presentation Flash Talks
1:10 PM - 2:00 PM	Lunch and Poster Session
2:00 PM - 2:30 PM	**Invited Talk: Dr. Alex Ramadan** Can perovskite semiconductors be more sustainable than conventional technologies?
2:30 PM - 3:00 PM	**Invited Talk: Dr. Baldeep Kaur** The Role of Sustainable Materials in Carbon Capturing

3:00 PM - 3:30 PM	**Invited Talk: Dr Wan Maryam Wan Ahmad Kamil** Developing Sustainable Random Lasers Through Semiconductor Nanotechnology
3:30 PM - 3:50 PM	**Afternoon Break**
3:50 PM - 4:20 PM	**Invited Talk: Prof. Kamal Vidanapathirana** Exploring Conducting Polymers as Efficient Electrodes in Supercapacitor Applications
4:20 PM - 4:50 PM	**Invited Talk: Prof. Kumudu Perera** Engineering Polymer Electrolytes for light weight, flexible and safer super capacitors
4:50 PM - 5:00 PM	**Poster Prize Giving and Closing Remarks**

Poster Presentations

Poster Board No.	First Name	Last Name	Organisation	Paper Title
1	Tugba	Akkas Boynuegri	University of St Andrews	Catalyst development for catalytic methane decomposition to co-synthesis of CNTs and low-carbon hydrogen
2	Aylin	Albayrak		Interface Optimization in CF/PEEK Composites via Functionalized Polyimide Sizing
3	Rafael	Aroso	University of Coimbra	Light-Activated Antimicrobial PLA-Curcumin Films for Surface Decontamination
4	Nilanthy	Balakrishnan	Keele University	Symmetric double-layer capacitor with natural rubber and sodium salt-based solid polymer electrolyte and reduced graphene oxide electrodes
5	Nilanthy	Balakrishnan	Keele University	Substrate-induced strain in molybdenum disulfide thin films grown by aerosol-assisted chemical vapour deposition
6	Caroline	Davies-Brooks	The CCDC	Accelerating Porous Materials Design and Development
7	Carolina	Domingos	University of Coimbra	Immobilized Photosensitizers onto Biopolymers for Reusable Photodynamic Therapy in Healthcare Applications
8	Marcus	Dykes	Keele University	Vibration spectrum of a finite string supported by a Winkler foundation
9	Rehmat	Goodwin	University of Sheffield	Unraveling the Impact of AEAPTMS Passivation on Heterogeneities and Charge Dynamics in Wide-Bandgap Perovskites: Insights from Kelvin Probe Microscopy
10	Shumaila	Parvez	Keele University	The Physiological And Biochemical Response Of Rice (Oryza Sativa L.) Seedlings To 2d Mxenes (Ti3c2tx)
11	Douglas	Penning		Optimisation of starch-gelatine film optical properties through the addition of papaya and cantaloupe purees under different processing temperatures
12	Mariette	Pereira	University of Coimbra	Sustainable Synthesis and Functionalization of Photosensitive Biodegradable Polymers for Antibacterial Applications
13	Grace Dansoa	Tabi	University of Sheffield	Organic Cation Engineering in 2D Perovskites: Unravelling the Role of MA^+ and FA^+ on Stability and Structural Evolution
14	Forward	Uruakpa	Keele University	Assessment of Solar Energy Potential and Forecasting Accuracy in a Maritime Temperate Climate: A Case Study of Stoke-on-Trent, UK

Invited Speakers

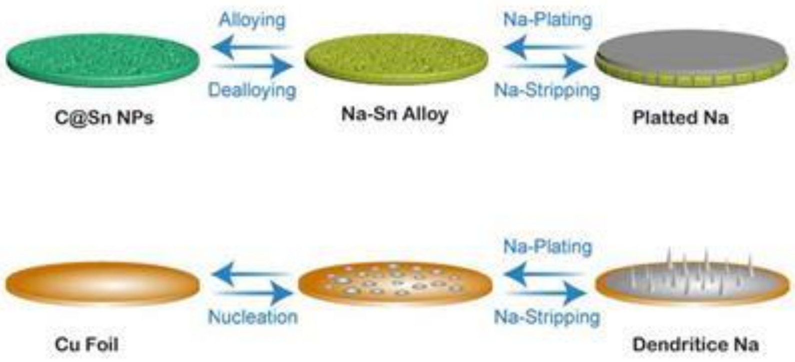
Development of Nucleophilic Metal-Seeded Anodes for Enhanced Sodium Metal Batteries

Dr. Zeeshan Ali
[1]*National University of Science and Technology, Pakistan*

Invited Talk: Dr. Zeeshan Ali, July 1, 2025, 12:15 - 12:45

Sodium metal batteries (SMBs) are emerging as a promising alternative to lithium-ion batteries due to their high theoretical capacity, cost-effectiveness, and the natural abundance of sodium. However, their practical application has been hindered by challenges such as dendrite formation and associated safety concerns. In this study, we introduce a free-standing film (FSF) embedded with nucleophilic tin (Sn) seeds within a porous carbon matrix (C@Sn FSFs) to address these issues. The Sn seeds facilitate uniform sodium nucleation, suppress dendrite growth, and enhance long-term stability during repeated plating and stripping cycles. Symmetric cells utilizing C@Sn FSFs demonstrated remarkable cycling stability over 2600 hours with an average Coulombic efficiency (CE) of 99.88%. Full cells paired with $Na_3V_2(PO_4)_3$ cathodes exhibited excellent cycling performance, superior rate capabilities, and delivered an energy density of 290 Wh/kg, underscoring their potential for scalable and efficient energy storage applications. Building on this approach, we developed a copper foam scaffold with large pores to prevent overcoating during the application of protective layers. Using a simple electrochemical deposition process, Sn metal seeds were embedded into the scaffold to create Cu_3Sn@Cu, followed by the optimization of the Sn seeds and an alloy interface to enhance seeding efficacy and nucleophilic properties. A protective Al_2O_3 coating was subsequently applied, and evaluations confirmed its ability to effectively mitigate dendrite formation. Symmetric cells using Al_2O_3-coated Cu_3Sn@Cu scaffolds achieved exceptional cycling stability, operating for over 8000 hours at 2 mA cm^{-2} and 4 mA h cm^{-2}. In-situ and ex-situ analyses revealed suppressed dendrite growth and the formation of a $Na_{15}Sn_4$ alloy, which reduced the nucleation barrier and improved deposition uniformity. The Al_2O_3 coating provided additional protection, enabling stable operation at high current densities without compromising ion transport. These findings demonstrate that the combination of nucleophilic seeding, intermetallic scaffolds, and inorganic protective coatings synergistically stabilizes SMBs, addressing key challenges of safety and long-term cycling stability. This work highlights the Cu_3Sn@Cu scaffold with a protective Al_2O_3 layer as a robust and scalable solution for high-performance SMBs, paving the way for the integration of advanced metallic and intermetallic frameworks in commercial energy storage applications.

Keywords: Interfacial alloys; nucleophilic seeding; conductive scaffolds; Na15Sn4 interface; dendrites suppression.



Alloying
Dealloying
Na-Plating
Na-Stripping
C@Sn NPs
Na-Sn Alloy
Platted Na
Na-Plating
Nucleation
Na-Stripping
Cu Foil
Dendritice Na

The Role of Sustainable Materials in Carbon Capturing

Dr Baldeep Kaur[1]
[1]University of Greenwich, United Kingdom

Invited Talk: Dr. Baldeep Kaur, July 1, 2025, 14:30 - 15:00

Carbon capturing utilisation and storage (CCUS) is a necessary step forwards to achieve the environmental sustainable development goals (SDG). Carbon capturing can be achieved either through chemisorption or physisorption mechanisms. A variety of materials and mechanisms are being researched to determine the efficiency of carbon absorption methods to achieve the environmental SDGs as the carbon capturing process requires to be efficient and effective. Several materials such as metal organic frameworks, carbon nanotubes, biochar, activated carbon, cement dust and other materials are being tested to establish the processes at pilot scale for industrial applications. This research focuses on the physisorption method of carbon capturing using the waste products of the cement industry – cement bypass dust and flue gases. Carbon absorption efficiency in physisorption mechanisms also depends on the available CO2 concentration, moisture content of bulk material, reaction time efficiency of a reactor, and temperature conditions. The changes in material properties during carbon capturing processes due to changes in moisture, temperature, increased residence time impacts the handleability of materials in bulk quantities. This research focuses on improving the carbon capturing efficiency, and improving the handleability of bulk materials at industrial scale.

Room Temperature Dipolar Excitons in van der Waals Heterostructures

Dr Abhishek Misra[1]
[1]IIT Madras, India

Invited Talk: Dr. Abhishek Misra, July 1, 2025, 10:00 - 10:30

Excitons are the bosonic system and thus the careful manipulation of their number density can lead to a range of many-body complexes. Excitons with permanent out-of-plane electric dipole moment interact via dipole–dipole interactions. Such excitons, known as interlayer excitons (IX) or dipolar excitons, further enrich the excitonic phase diagram depending on the nature of the dipole-dipole interaction. These appealing dipolar interactions have been the subject matter of intense investigations since decades using GaAs/AlGaAs quantum well structures. With the advent of van der walls heterostructures, the realization of dipolar excitons, at least theoretically, has become rather easy. Experimentally, these have been confirmed via luminescent emission in the heterostructures of transition metal dichalcogenides. However, in these heterostructures, the IXs are not always observed as the emission is very sensitive to the lattice mismatch and the twist angle between the constituent materials. Moreover, their emission intensity is very feeble compared to corresponding intralayer excitons at room temperature. In this talk, I will discuss a possible way to stabilize these IX at room temperature. Room temperature stabilization of the dipolar excitons holds significance not only to explore many-body physics at elevated temperatures but also for their applications in the field of quantum technologies.

Ref: Saroj Poudyal et al., Nano Lett. 2024, 24, 9575−9582.

Atomically Thin Semiconductors for Science and Technology

Professor Amalia Patane[1]
[1]*University of Nottingham, United Kingdom*

Invited Talk: Prof. Amalia Patane, July 1, 2025, 09:30 - 10:00

Atomically-thin semiconductors, also called two-dimensional semiconductors (2DSEM), behave in a fundamentally different way from their bulk (3D) counterparts and their unique electronic properties can support entirely new effects at the atomic scale. 2DSEM can advance fundamental science and represent a front-runner technology for building a sustainable semiconductor industry, reducing the electricity demand in high-performance computing and AI.

In this presentation, I will discuss scientific and technological challenges in the field, and present novel approaches to the development of 2DSEM. Following the presentation of a bespoke facility at Nottingham for the integration of epitaxial growth with advanced studies by scanning probe microscopy and electron spectroscopy in ultra-high vacuum [1-2], I will introduce new 2DSEM and discuss the precise engineering of these materials, pushing the limits of what can be created, probed and exploited [2-3]. Finally, I will introduce our EPSRC Programme Grant (NEED2D 2025-30), which brings together many research institutions and industry to develop prototype low-energy-consumption 2DSEM electronics beyond traditional systems.

[1] https://bit.ly/3zN0Odx
[2] https://www.youtube.com/watch?v=GHCxEDMh3R0

Engineering Polymer Electrolytes for light weight, flexible and safer super capacitors

Prof. Kumudu Perera[1]
[1]Wayamba University of Sri Lanka, Sri Lanka

Invited Talk: Prof. Kumudu Perera, July 1, 2025, 16:20 - 16:50

Today, the demand for power has exceeded the generation due to proliferation of diverse devices that require uninterrupted power. This situation together with the endangering state of fossil fuels and identification of its adverse effects have made a massive attraction on renewable energy sources. Due to their intermittent nature, energy storage has become vital in order to supply continuous power. Even batteries and capacitors have been recognized as good energy storage devices, there exists a controversial between power and energy of those devices. Super capacitors have been able to bridge that gap exhibiting higher power and energy than batteries and conventional capacitors respectively. Due to growing popularization in diverse applications with different design demands, dimension limitations, light weight requirements as well as user friendliness, there exists a keen interest to develop super capacitors with light weight, flexibility and assured safety. One approach is developing the electrolyte of a supercapacitor which plays an instrumental role. At the stage of inception, many of the super capacitors were having liquid electrolytes both in aqueous and non-aqueous form. However, the conventional and usual drawbacks have promoted the search for solid and gel type electrolytes based on different polymers, salts. Initial polymer electrolytes had low ionic conductivities and poor mechanical properties restricting super capacitor applications greatly. Due to continuous progress, diverse modified polymer electrolytes like gel polymer electrolytes have been explored with conductivity values identical or higher than liquid electrolytes while acquiring a high demand for super capacitors. In recent years, several bio polymer-based electrolytes, ionic liquid-based electrolytes have shown promising features to serve in super capacitors. While reducing the weight of the device, it has been possible to leverage flexibility and safety. However, it is still needed to explore solutions for issues like high internal resistance, moderate durability and limited potential windows. However, upon the outcomes present today, it can be stated that polymer electrolytes are viable candidates as super capacitor electrolytes. Traversing modifications further is highly essential to capture optimum performance of super capacitors while assuring light weight, flexibility and safety.

Can perovskite semiconductors be more sustainable than conventional technologies?

Dr Alex Ramadan[1]
[1]University of Sheffield, United Kingdom

Invited Talk: Dr. Alex Ramadan, July 1, 2025, 14:00 - 14:30

Metal halide perovskites are an exciting emerging semiconductor technology which have been the subject of intense research efforts in the photovoltaic and optoelectronics research community for over a decade. As semiconductors, they are unusual due to their impressive defect tolerance, tunable bandgaps, and excellent optoelectronic properties. These properties have led to unprecedented developments in single junction photovoltaics where their power conversion efficiencies now rival those achievable with crystalline silicon. In addition to their successful demonstration in photovoltaics, perovskite semiconductors have shown great promise in photodetectors, transistors and as the emitting layer in light emitting diodes.
From a sustainability perspective these semiconductors are interesting as they can be made from earth abundant materials and through less energy intensive fabrication processes than traditional semiconductors. In this talk I will introduce our research on perovskite semiconductors. I will present our recent work investigating aspects of their sustainability and outline how we can incorporate considerations around sustainability in future research.

Exploring Conducting Polymers as Efficient Electrodes in Supercapacitor Applications

Prof. Kamal Vidanapathirana[1]
[1]*Wayamba University of Sri Lanka, Sri Lanka*
Invited Talk: Prof. Kamal Vidanapathirana, July 1, 2025, 15:50 - 16:20

Supercapacitors are emerging as critical components in the landscape of advanced energy storage due to their high power density, rapid charge/discharge capability, and long cycle life. Among the various electrode materials under investigation, conducting polymers (CPs) have garnered significant attention because of their unique combination of redox activity, electrical conductivity, and mechanical flexibility. This presentation provides the role of conducting polymers—such as polyaniline (PANI), polypyrrole (PPy), and polythiophene (PTh)—as electrode materials in supercapacitors. It delves into their charge storage mechanisms, key advantages, and the challenges associated with stability and cycling performance. Recent advancements in hybrid materials and nanostructured architectures are discussed as strategies to overcome these limitations and enhance electrochemical performance. The talk concludes with a look toward future trends, including the development of sustainable, flexible, and scalable energy storage systems incorporating CPs. The presentation aims to provide a comprehensive overview of how conducting polymers can contribute to the next generation of high-performance, low-cost supercapacitors.

Developing Sustainable Random Lasers Through Semiconductor Nanotechnology

Assoc Prof Ts Dr Wan Maryam Wan Ahmad Kamil[1]
[1]*University Sains Malaysia, Malaysia*
Invited Talk: Dr Wan Maryam Wan Ahmad Kamil, July 1, 2025, 15:00 - 15:30

Random lasing or an open cavity laser system utilises nanostructures to sustain the light long enough for amplification and lasing to occur by manipulating the refractive index of the structures. Engineering these structures to confine the light has led to achieving lasing without the need of conventional mirrors. Fabricating the gain medium at reduced dimensionality (sub-micron scale) makes it appealing for small scale devices. Ideally, low-cost illumination sources with high brightness and low spatial coherence are preferred for imaging of biological tissues, hence, random lasers are good candidates due to its low spatial coherence. However, current random lasers for this application utilise dyes as a gain medium. The major drawback is dye degradation and photobleaching which means that the dye gain medium can only be used once and must be replaced at each excitation. In addition, existing random lasers commonly operate in the spectral range of ~1-2 microns that cannot provide a resolution good enough for bio-imaging. To overcome this technological limitation, a stable and sustainable gain medium emitting in the UV wavelength is key.

Since 2017, we have identified a promising candidate as a UV random laser gain medium by utilising zinc oxide (ZnO) nanostructures. The lasing threshold as low as 0.07 W/cm2 which was two orders of magnitude less than for laser dyes [1]. The main challenge is its high threshold since it is an open cavity system. One proven method of reducing the lasing threshold was achieved by designing the ZnO random laser with specific dimensions and doping with Aluminium [2]. To utilize the random lasing emission in current bio-imaging systems, it is also crucial to develop fibre based random lasers. A fibre based random laser designed within the UV range is most beneficial as biosensors. This talk will highlight ZnO random laser characteristics with and without doping, its capability as a nanosensor and the experiments recently carried out towards implementing a fibre based random laser using ZnO as the gain medium. Observation of stable emission and differences on threshold behaviour that is dependent on ZnO morphology will be discussed. In addition, investigation on tuneable random lasers will also be included.

[1] N. Fadzliana, S. A. M. Samsuri, S. Y. Chan, H. C. Hsu, and W. Maryam, “Influence of Al doping on random lasing in ZnO nanorods,” Opt Laser Technol, vol. 124, p. 106004, Apr. 2020, doi: 10.1016/j.optlastec.2019.106004.
[2] A. T. Ali et al., “UV random laser in aluminum-doped ZnO nanorods,” Journal of the Optical Society of America B, vol. 38, no. 9, p. C69, Sep. 2021, doi: 10.1364/JOSAB.427132.

Clean interfaces on 2D semiconductors

<u>Dr Yan Wang</u>[1]
[1]University of Cambridge, United Kingdom

Invited Talk: Dr. Yan Wang, July 1, 2025, 10:30 - 11:00

Two dimensional (2D) semiconductors, specifically monolayer transition metal dichalcogenides (TMDs), have attracted tremendous interest due to their fundamental merits in transistor scaling. However, the main challenge for realizing high performance field effect transistors (FETs) on monolayer TMDs is that the atomically thin TMDs are very sensitive to any perturbation at the metal/semiconductor and semiconductor/dielectric interfaces. In this talk, I will briefly introduce our work on realizing clean van der Waals contacts for high-performance N-type and P-type FETs on atomically thin TMDs. Using scanning transmission electron microscopy imaging and X-ray photoemission spectroscopy, we show that the atomically sharp metal/semiconductor interfaces with no detectable chemical interaction between the metals and TMDs are preferred. Further, I will discuss our recent work on investigating how the interface interactions between monolayer TMDs and dielectrics influence the device performance.

Contributed Speakers

Effect of Te substitution and copper vacancies on the thermoelectric performance of BiCuSeO

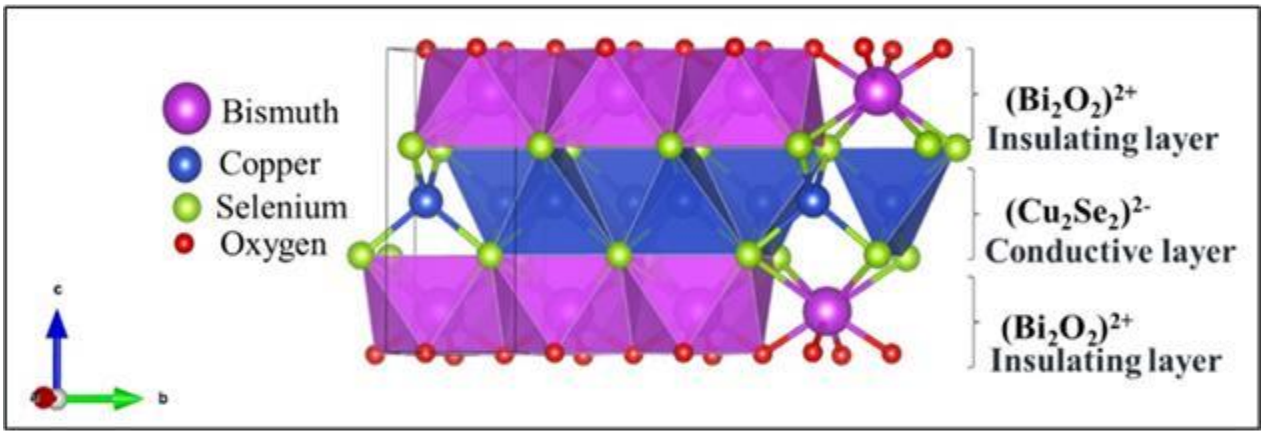
Dr Deepa Bhatt[1], Paz Vaqueiro[1], Anthony Powell[1]
[1]University of Reading, United Kingdom

Oral Contributions, July 1, 2025, 11:15 - 12:15

The decline in fossil fuels and rising CO_2 emissions demands efficient and sustainable solutions. Thermoelectric (TE) technology offers a way to generate electricity from waste heat, facilitating reduction in carbon emissions. TE performance is measured by the dimensionless figure of merit ZT, which reflects their electrical and thermal transport efficiency. Recently, layered oxychalcogenides have emerged as promising candidates for high-performance thermoelectric applications, owing to their distinctive crystal structure composed of alternating oxide and chalcogenide layers. This architecture offers a unique blend of thermal and electrical transport properties. BiCuSeO, a p-type oxychalcogenide, has a potential to exhibit a high figure of merit (ZT ≈ 1.5 at 873 K) and ultralow thermal conductivity (~0.5 $W{\cdot}m^{-1}{\cdot}K^{-1}$) 1 [1]. In this study, we have explored the substitution of Se by Te, as a route to increase the covalency of the chalcogenide [Cu2Se2]2- layers and hence increase the electrical conductivity. $BiCu_{1-y}Se_{1-x}Te_xO$ compositions ($0 \le y \le 0.1$, $0 \le x \le 0.4$) were synthesized using high-temperature solid-state reaction. Powder X-ray diffraction and neutron scattering were employed for phase identification and detailed structural characterization. Measurements of thermal and electrical transport properties were performed as a function of composition. Our data show that Te substitution reduces thermal conductivity by approximately 20%. Introducing Cu deficiency significantly improves the electrical transport behaviour and overall thermoelectric performance. These findings offer insights into the optimisation of the performance of oxychalcogenide-based thermoelectric through compositional engineering.

References:

[1] S. Tippireddy, ACS Appl. Energy Mater., vol. 4, no. 3, pp. 2022–2040, 2021.



Assessing the discharge-recharge mechanism of monovalent cation-directed hausmannite Mn_3O_4 cathodes in aqueous Zn-ion batteries

Melanie Randall-Evans[1], Guanjie He[1,2], Ian Scowen[1], Tasnim Munshi[1], Filipe Marques Mota[1]
[1]University of Lincoln, United Kingdom, [2]University College London, United Kingdom

Oral Contributions, July 1, 2025, 11:15 - 12:15

As the energy density capabilities of lithium–ion batteries reach theoretical limits, alternative technologies are more urgent than ever. Multivalent-ion counterparts utilising multiple-charge carriers have long been tipped as a solution. In particular, divalent Zn–ion presents a cost-effective alternative, largely due to the abundancy of zinc in the Earth's crust, the promise of fast charge-discharge capabilities, and a high-energy safe metal anode allowing the use of inexpensive aqueous electrolytes. However, state-of-the-art Mn-based cathode materials required for these cells possess poor stability throughout cycling, limiting the possible commercialisation.
To tackle these limitations, manganese oxide active materials were synthesized using $Mn(NO_3)_2 \cdot 4H_2O$ and a Na/K/Cs hydroxide precursor (at varying concentrations), through a cost-effective low-temperature sol-gel synthesis. The resulting crystal structures examined by XRD were confirmed to be hausmannite Mn_3O_4, with the monovalent cations present in varying concentrations recorded through EDX and ICP analysis. Aqueous Zn–ion batteries were then assembled, pairing the prepared cathode materials with a Zn metal plate in an aqueous zinc sulphate electrolyte. The effects of the selected monovalent cations under optimised concentrations were reflected in the achieved cell capacities, with Na-directed Mn_3O_4 delivering a capacity of ca. 200 mAh/g in the 2nd cycle, at 100 mA/g.
Subsequently, the transition during cyclling from a one-stage to a stable two-stage discharge mechanism with increasing capacities was investigated through cyclic voltammetry and XRD analyses of spent cathodes. This work significantly builds upon the current Zn–ion literature, uncovering the underlying electrochemistry of Mn-based cathodes towards long-term practicality.

Tailoring optical and thermal properties in rare-earth doped MoS_2 for device applications

Dr Geeta Sharma[1], SarathKumar Loganathan[1], EricKumi Barimah[1], Chun Wang[1], Animesh Jha[1]
[1]*University Of Leeds, United Kingdom*

Oral Contributions, July 1, 2025, 11:15 - 12:15

This study explores the structural, optical, and thermal properties of ytterbium-doped molybdenum disulfide (MoS_2:Yb^{3+}) thin films synthesized via femtosecond pulsed laser deposition (fs-PLD) across a controlled thickness range of 1–10 nm. Comprehensive characterization using X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), Raman spectroscopy, and photoluminescence (PL) reveals pronounced thickness-dependent behavior in crystallinity, phonon dynamics, and carrier recombination. Ultrathin films (~1.8 nm) exhibit enhanced radiative efficiency (PL lifetime ~0.012 ms), attributed to reduced defect density, whereas thicker films (~10.2 nm) display longer lifetimes (~0.019 ms) and improved crystallinity due to strain relaxation and stronger interlayer coupling. Temperature-dependent Raman spectroscopy highlights Yb^{3+}-induced phonon anharmonicity, with a lower in-plane E_2g^1 temperature coefficient ($\alpha = -0.0128\ cm^{-1}/°C$) compared to pristine MoS_2, indicating strain compensation. Conversely, the out-of-plane A_1g mode exhibits a higher coefficient ($-0.0186\ cm^{-1}/°C$), suggesting enhanced interlayer charge transfer. Phonon lifetime-based thermal conductivity estimation ($\kappa \approx 66 \pm 6$ W/m·K) reveals a reduction relative to undoped MoS_2 due to increased phonon scattering from Yb^{3+} dopants. These findings underscore the tunable optoelectronic properties of MoS_2:Yb^{3+} thin films, with thinner films suitable for high-speed optoelectronic applications such as light-emitting devices, and thicker films offering advantages for thermal management and photovoltaic systems. The work provides new insights into defect engineering, electron–phonon interactions, and the role of rare-earth doping in 2D materials, highlighting their potential in next-generation energy and photonic devices.

Sustainable liquid phase exfoliation processes for 2D materials using predictive models and feedstock re-use

Jacob Brown[1], Diego Perez-Alvarez[1], Dr Jason Stafford[1]
[1]*University Of Birmingham, United Kingdom*

Oral Contributions, July 1, 2025, 11:15 - 12:15

The use of mechanical force to synthesise graphene and other two-dimensional materials has provided an opportunity to create sustainable processes and avoid the introduction of defects that adversely impact functional properties. Despite the inherent scalability of liquid phase exfoliation methods, there are open challenges around obtaining an accurate description – to enable process and material property optimisation – and limiting the substantial volumes of waste feedstock produced. This work presents two complementary research avenues from our collaborative activities towards this aim of obtaining truly sustainable 2D materials technologies [1,2].

An important factor is the ability to forecast material production. By monitoring changes in the distribution of graphite particles as they undergo breakup during liquid-phase exfoliation, we show that statistical population balance models (PBM) are a feasible solution for establishing yield and future production of graphene nanosheets. A combination of experimental measurements are used to recover the material distribution and fit the PBM over all scales respectively. This fitted PBM can then provide insights on the breakage mechanisms underpinning the exfoliation process and examine production over time.

Using the same shear exfoliation method, and MoS_2 as the prototypical material, we then demonstrate a sustainable approach to recover and reuse unexfoliated precursor material and the exfoliation solvent to reduce waste by up to 82% and solvent requirement by up to 72%. Importantly, both predictive modelling and feedstock recycling can be scaled and immediately implemented using existing infrastructure.

[1] https://doi.org/10.1016/j.carbon.2024.119687, Carbon, 231, 119687, 2025.
[2] https://doi.org/10.1021/acssuschemeng.4c05845, ACS Sustainable Chem. Eng., 12(39), 14363–14370, 2024.

Poster Presentations

Catalyst development for catalytic methane decomposition to co-synthesis of CNTs and low-carbon hydrogen

Tugba Akkas Boynuegri[1]
[1]University Of St Andrews, United Kingdom

Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

In this study, carbon nanotubes (CNTs) and hydrogen were synthesized by the catalytic methane decomposition in the presence of nickel based catalyst. Principally, this research involves three main steps: catalyst preparation, testing its performance, and the characterization of the final product of CNTs. For catalyst preparation, the impregnation method was selected and applied for MgO support. Then, methane decomposition reaction was performed in a quartz tube reactor to test its performance under constant methane and nitrogen gas flow at 650 °C. Hydrogen synthesis and CNTs growth on the catalyst were proved and characterized by GC, SEM, TEM, RAMAN, and TGA analysis.

Interface Optimization in CF/PEEK Composites via Functionalized Polyimide Sizing

__Aylin Albayrak__[1], Kadir Turhan[2], Mustafa Çakır[3], Tony McNally[1]
[1]United Kingdom, [2]Türkiye, [3]Türkiye

Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Carbon fiber reinforced PEEK composites are increasingly used in aerospace, automotive, sports equipment, and renewable energy applications thanks to their exceptional strength, lightweight nature, and resistance to harsh environments. Polyimides and their composites have been recognized as one of the most promising engineering plastics of the twenty-first century due to their high-performance, superior mechanical properties, thermal stability and chemical resistance [1]. Diamine and dianhydride monomers are used in the synthesis of polyimides which takes place in two steps firstly the synthesis of soluble and processable high molecular weight polyamic acid. The second step is the cyclodehydration of polyamic acid by a suitable method (thermal or chemical imidisation) to obtain polyimides by ring closure [2].
The aim of this study was to synthesise a novel polyimide (PI) to improve the interfacial bonding and adhesion between carbon fibre (CF) and poly-ether-ether-ketone (PEEK), a high-performance engineering polymer. For this reason, a new diamine and dianhydride were synthesised and the structure of all monomers was confirmed by FTIR and 1H NMR spectroscopy. Then the polyimide was combined with different percentages of reduced graphene oxide (rGO) in resin form. In this way, it was coated on to CF by thermal imidisation in an oven at about 300 o C. CF-PEEK composite materials with different percentages of rGO /PI sizing agent produced. The thermal, mechanical and thermomechanical properties of these composites was measured. It was determined that the synthesised sizing agent significantly improved the performance at the CF-PEEK interface and is promising for further studies.

Light-Activated Antimicrobial PLA-Curcumin Films for Surface Decontamination

Rafael T. Aroso[1], Carolina V. Domingos[1], Madalena F.C. Silva[1], João R.A. Pires[2], Mariette M. Pereira[1]
[1]CQC-IMS, Department of Chemistry, University of Coimbra, Portugal, [2]Bio4Plas – Biopolimeros, Lda., Portugal

Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

The rise of multi-drug resistant (MDR) bacteria, responsible for over 1.3 million deaths annually, poses a major health challenge. Contaminated hospital surfaces and medical devices are key contributors to the spread of MDR infections, highlighting the urgent need for effective and safe disinfection strategies. Current disinfectants such as ethanol, bleach, and UV light have notable drawbacks, including toxicity, limited efficacy, and resistance development. An emerging alternative is photodynamic inactivation (PDI), which uses light-activated photosensitizers (PS) to generate reactive oxygen species that inactivate bacteria. In this study, we developed a novel photodecontaminating material by embedding the natural, non-toxic PS curcumin into a biodegradable polylactic acid (PLA) matrix. Using a solvent casting method, we obtained PLA films containing 15% curcumin and characterized their properties with techniques such as DSC, TG, PLTM, FTIR, and XRPD. When exposed to blue LED light (32.9 J/cm^2), the PLA-curcumin films achieved a 99.99% reduction in Staphylococcus aureus, demonstrating strong antimicrobial activity. Additionally, the films inhibited fungal growth on raspberries under white light, indicating their potential for food packaging applications. With their biocompatibility, light-activated antimicrobial properties, and versatility, PLA-curcumin films represent a promising solution for reducing microbial contamination on surfaces in medical and food-related settings.

Acknowledgements: Fundação para a Ciência e Tecnologia(FCT), QREN/FEDER for Projects UIDB/00313/2020, UIDP/00313/2020 and COMPETE2030-FEDER-00882400 for project 276/UID/2025/CD. They thank UC-Santander for "PhotoBioSyn" SeedProjects@UC 2024 funding. Furthermore, they thank project nº 6979 - PRODUTECH R3 [Recuperação-Resiliência-Reindustrialização financed by PRR - Recovery and Resilience Plan and by the European Union Next Generation EU Funds.

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

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

In recent years, natural polymers have received tremendous attention due to the latest advances in green technology for a sustainable future. Herein, solid polymer electrolytes (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 (σ_RT) of 7.52 × 10-4 S/cm. This optimized electrolyte is purely an ionic conductor with an activation energy (Ea) 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 (Csc) 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-1 shows a fast drop of single electrode specific discharge capacitance (Csd) at the beginning, but it started to saturate after the 5,000th cycle proving the good stability of the supercapacitor. These findings are relevant to expanding the functionalities of supercapacitors having natural rubber-based SPEs in green technologies.

Reference

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

Substrate-induced strain in molybdenum disulfide thin films grown by aerosol-assisted chemical vapour deposition

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Transition metal dichalcogenides have been extensively studied in recent years due to their fascinating optical, electrical, and catalytic properties. However, low-cost, scalable production remains a challenge. Aerosol-assisted chemical vapour deposition (AACVD) is a solution-based process that provides a new method for scalable thin film growth. In this study, we demonstrate the growth of molybdenum disulfide (MoS2) nanostructures using AACVD method. This method proves its suitability for low-temperature growth of MoS2 nanostructures on various substrates, including glass, silicon dioxide, quartz, silicon, hexagonal boron nitride, and highly ordered pyrolytic graphite. The as-grown MoS2 shows evidence of substrate-induced strain [1]. The type of strain and the morphology of the as-grown MoS2 highly depend on the growth substrate's surface roughness, crystallinity, and chemical reactivity. Moreover, the as-grown MoS2 shows the presence of both direct and indirect band gaps, suitable for exploitation in future electronics and optoelectronics.

Reference

[1] L. J. Adams, P. D. Matthews, J. M. Morbec, N. Balakrishnan, Substrate-induced strain in molybdenum disulfide grown by aerosol-assisted chemical vapor deposition, Nanotechnology, 35, 395602 (2024).

Accelerating Porous Materials Design and Development

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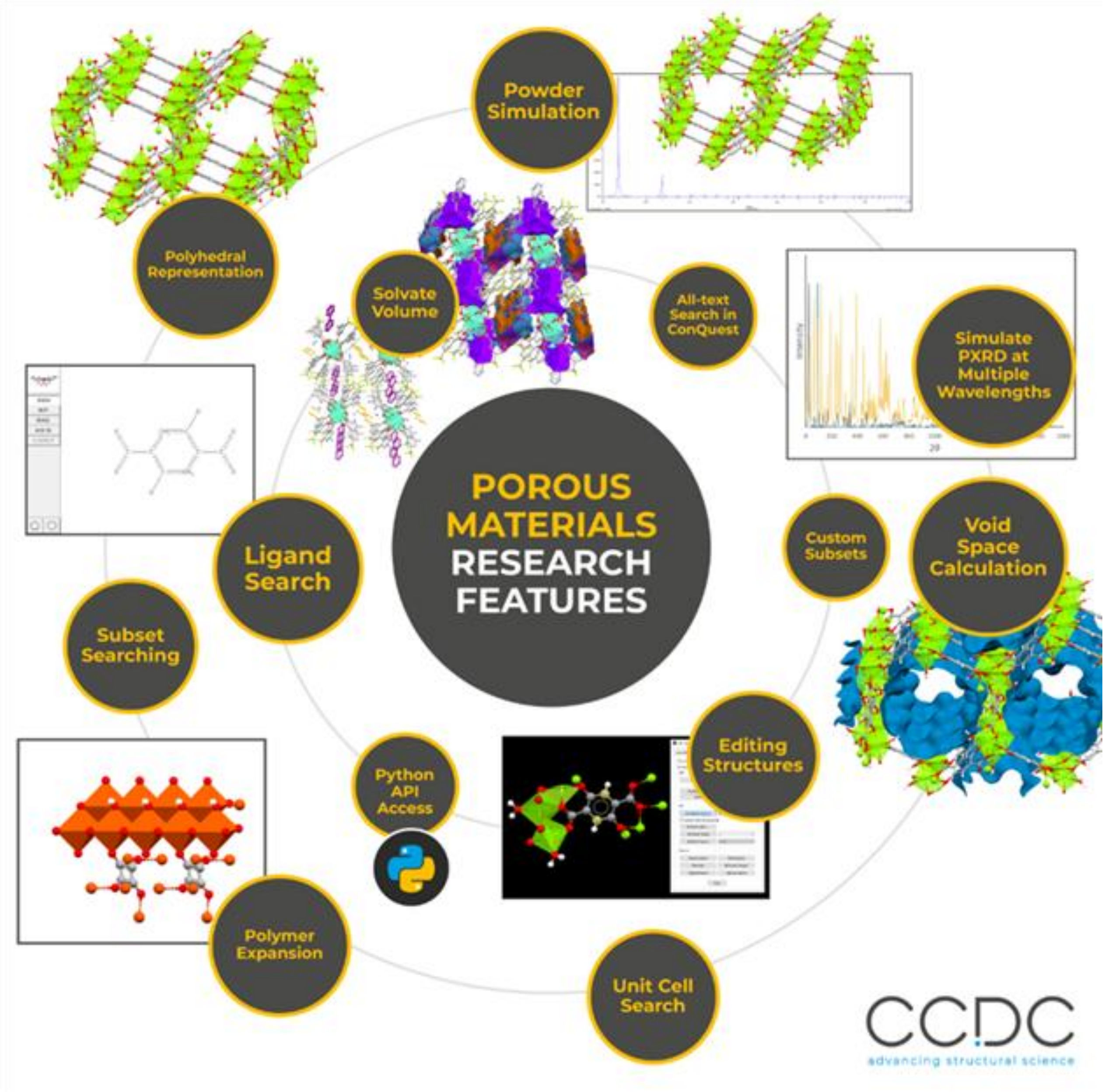
Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Metal-organic frameworks (MOFs) are crystalline solid-state materials comprised of metal-ion clusters linked by organic ligands to form 1D, 2D or 3D topologies. MOFs which exhibit considerable void volumes are of particular interest for their applications in a wide variety of uses such as carbon capture, drug delivery, chemical separations, catalysis and atmospheric moisture harvesting. As with other materials, the design of MOFs with specific physical and chemical properties in mind has recently been accelerated using digital tools combined with an increasingly sophisticated understanding of structure-property relationships.

The Cambridge Structural Database (CSD) has over 130 000 experimentally determined MOF structures. The Cambridge Crystallographic Data Centre (CCDC), which houses The CSD, has a portfolio of software designed to facilitate the analysis of MOFs in the context of this wealth of structural data.

This poster presents a streamlined workflow for using The CSD to explore the MOF structures, including visualisation, void & pore analysis, guest molecule identification and literature review to support data-driven design and discovery of functional materials.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Void Space Calculation
Subset Searching
Editing Structures
Python API Access
Polymer Expansion
Unit Cell Search
CCDC
advancing structural science

Immobilized Photosensitizers onto Biopolymers for Reusable Photodynamic Therapy in Healthcare Applications

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Multidrug-resistant (MDR) bacteria cause an estimated 1.3 million deaths annually, with contaminated surfaces in healthcare settings serving as major vectors of transmission, particularly for vulnerable patients and staff. Simultaneously, plastic waste—much of it from disposable, non-biodegradable medical products—poses a significant environmental threat.Addressing both issues, photodynamic therapy (PDT) offers a sustainable, residue-free antimicrobial strategy via light-activated surfaces.

We report biodegradable films composed of polylactic acid (PLA) functionalized with a novel mono-cationic imidazolium porphyrin as an immobilized photosensitizer. These films exhibit strong photostability, mechanical durability, and are designed for repeated use. When illuminated with blue light (16–24 J/cm^2), the PLA–porphyrin films achieved complete inactivation (>7-log reduction) of both antibiotic-sensitive and MDR strains of Staphylococcus aureus and Escherichia coli. Our results highlight the promise of combining biodegradable polymers with light-responsive agents to develop reusable, non-toxic antimicrobial materials. These systems not only help reduce the spread of infections and antimicrobial resistance but also offer an eco-friendly alternative to conventional disinfectants and single-use plastics in healthcare.

Acknowledgments:
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Vibration spectrum of a finite string supported by a Winkler foundation

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

This problem investigates the linear vibrations of an elastic string supported by a Winkler-type elastic foundation, with boundary supports featuring both positive and negative stiffness setups. The latter may arise in mechanical meta-materials. The presence of the elastic foundation under associated boundary conditions creates qualitative shifts in the eigenmode behaviour. Specifically, we identify trapped modes spatially confined near the ends of the string. This discovered localised dynamic behaviour may lead to new developments in vibration isolation and wave filtering in structured environments. Additionally, we derive a three-term asymptotic expansion for the high-frequency eigenvalues, starting from the exact transcendental equation, providing an analytical insight into the studied vibration spectrum. The derived asymptotic formulae are validated by comparison with numerical solutions. The obtained results have potential to be used in the design of tunable resonant mechanical systems, acoustic metamaterials, and elastic waveguides.

Unraveling the Impact of AEAPTMS Passivation on Heterogeneities and Charge Dynamics in Wide-Bandgap Perovskites: Insights from Kelvin Probe Microscopy

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Heterogeneities introduced during the fabrication of perovskite semiconductors impact device performance and stability by influencing charge dynamics across multiple length scales. Kelvin probe microscopy (KPFM) allows us to study heterogeneities in surface photovoltage and correlate them to changes in morphology. Surface passivation is widely used to reduce defects and improve homogeneity in perovskite semiconductors. A recent science paper by Hung-Lin et al demonstrated a new surface passivation molecule (AEAPTMS) which reduces heterogeneities in perovskite semiconductors of several bandgaps and results in solar cells with exceptional open-circuit voltages. I will present our work using KPFM to study the impact of this surface passivation on the morphology and surface photovoltage of a wide bandgap perovskite semiconductor, $Cs_{0.15}FA_{0.85}Pb(I_{0.16}Br_{0.4})_3$, with a bandgap relevant for perovskite on silicon tandem photovoltaics (1.77eV). We study the surface photovoltage of our perovskite system under broad spectrum white light illumination as well as above and below band gap illumination observing clear differences between passivated and unpassivated perovskites demonstrating the functionality of AEAPTMS as a passivation layer on multiple length scales. Finally, I will discuss strategies and important optimisation approaches needed to conduct KPFM studies on challenging materials.

THE PHYSIOLOGICAL AND BIOCHEMICAL RESPONSE OF RICE (ORYZA SATIVA L.) SEEDLINGS TO 2D MXENES (TI3C2TX)

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Two-dimensional (2D) materials are a novel class of nanomaterials, showing applications in nanotechnologies. MXenes ($Ti_3C_2T_x$) are one of the members of the 2D materials family. A very limited studies have examined the impact of these 2D nanomaterials on green plants. The lethal effects of $Ti_3C_2T_x$ on plant health require careful examination. Rice is a crucial staple crop around the world. In this work, 2D $Ti_3C_2T_x$ nanosheets were synthesised by etching Al from Ti_3AlC_2 and characterised by SEM, EDX, XRD, Raman and FTIR spectroscopy to confirm their morphology and chemical composition (see Figure 1). Four different suspensions of $Ti_3C_2T_x$ (25, to 100 μg/mL) were prepared and applied to rice seedlings. Growth-related traits and toxicity analyses were carried out after 8 days of treatment. Results demonstrate that the highest dosage of $Ti_3C_2T_x$ (100 μg/ml) decreased the germination percentage (GP), vigour index (VI), root length (RL), shoot length (SL) and chlorophyll contents (Chla, Chlb, Chlab) by 1.4%, 5.6%, 3.7%, 4.2% and (1.4%, 2.1% and 1.9%) ($p < 0.05$), respectively. These findings were correlated with oxidative damage caused by the highest level of $Ti_3C_2T_x$, as evidenced by the expression of antioxidant enzymes. At 100 μg/ml, the H_2O_2 and SOD (examined using spectrophotometric assay by measuring absorbance at 390 nm and 560 nm, respectively) increased by 2.7% and 11.9% ($p < 0.05$), respectively. Our results indicate that high concentrations of $Ti_3C_2T_x$ cause oxidative stress, which hinders rice seedlings' growth. Emphasis should be given in the future to manage the soil/plant interactions with $Ti_3C_2T_x$ carefully.

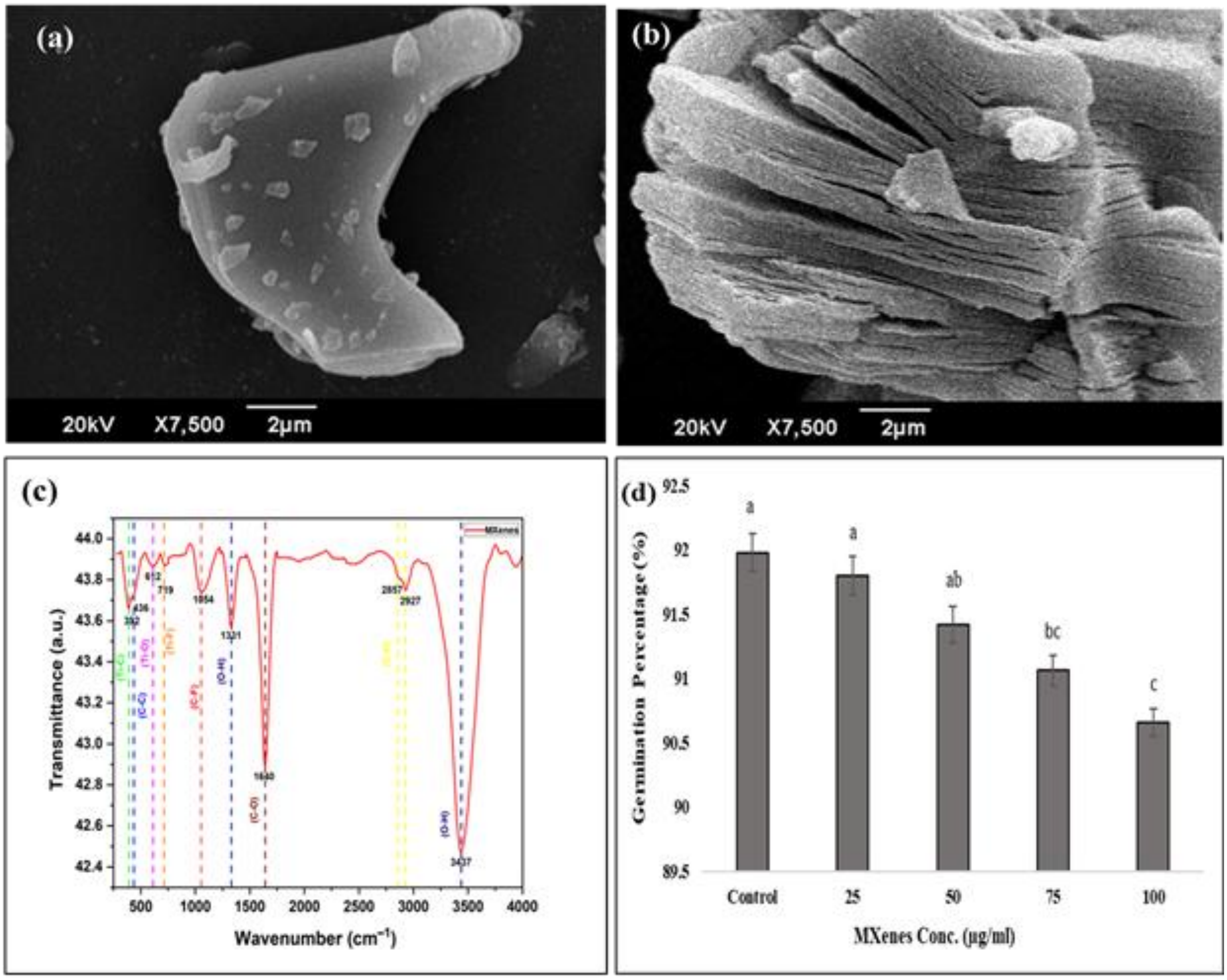

Fig 1. SEM images of (a) Ti_3AlC_2 (MAX phase) and (b) $Ti_3C_2T_x$ (MXenes). (c) FTIR spectra of $Ti_3C_2T_x$. (d) Effects of $Ti_3C_2T_X$ levels on the germination percentage (%) of the rice seedlings. The result represents the mean ± SE of five independent replications. Lowercase letters specify statistically significant variations between treatments at $p < 0.05$.

Optimisation of starch-gelatine film optical properties through the addition of papaya and cantaloupe purees under different processing temperatures.

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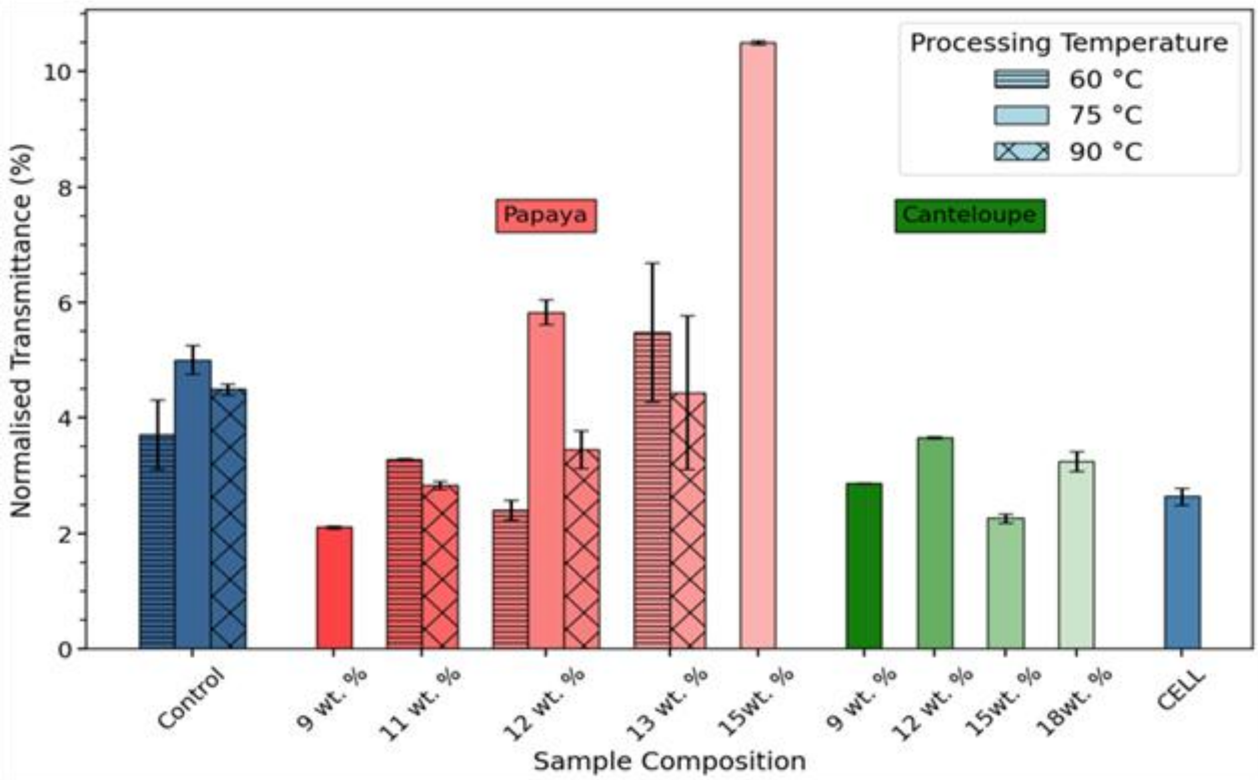
Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Starch-gelatine films are commonly utilised biodegradable alternatives to the petroleum-based polymers used for the packaging and preservation of foods. Whilst easily producible these films have poor optical properties thus reducing the visual appeal and saleability of products. Initial research has been conducted into improving the visible light transmittance of films whilst maintaining mechanical strength, using carotenoid groups, enzymes and fibre present in papaya purees. This study seeks to find an optimised composition, maximising optical transparency whilst maintaining mechanical strength and biodegradability. Through the addition of both papaya and cantaloupe purees under varying processing temperatures, it was found that a composition containing 12 wt. % papaya, produced at 75 °C was optimal. Visible light transmittance was increased by 16.36 ± 7.24 %, with a 9.83 ± 2.31 MPa Youngs Modulus and 52.53 ± 20.21 % elongation at break.

Through this study a positive correlation between visible light transmittance at λ = 500 nm and papaya concentration was determined. Transmittance of papaya-containing films exhibited a critical transition at ~13 wt.%, with higher concentrations displaying improved transparency. Conversely no statistically significant trend in transmittance was seen with respect to cantaloupe content. The sample with highest normalised transmittance was found to be 15 wt. % papaya produced at 75 °C at 10.51 ± 0.036 %, though with significantly reduced mechanical integrity.



Sustainable Synthesis and Functionalization of Photosensitive Biodegradable Polymers for Antibacterial Applications

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Photosensitive polymers have garnered significant attention due to their wide-ranging applications in electronics and medicine. Among them, polycarbonates are particularly notable for their exceptional properties, including optical clarity, heat resistance, high impact strength, dimensional stability, low water absorption, ease of sterilization, biocompatibility, and biodegradability, making them a superior alternative to conventional PVC-based polymers. Polycarbonates can be sustainably synthesized through the catalytic copolymerization of epoxides and carbon dioxide (CO_2), offering a greener route that avoids hazardous reagents such as phosgene. This method not only reduces environmental impact but also improves atom economy.
In this work, we report our recent progress in the development of photosensitive polymeric materials via catalytic copolymerization of CO_2 with vinyl epoxides. The resulting vinyl polycarbonates were subsequently functionalized at the C=C double bond through hydroformylation or bromination (Br_2 addition). These post-polymerization modifications enable fine-tuning of the physical and chemical properties of the materials. The resulting photosensitive polymers were evaluated for their photoinactivation efficacy against Staphylococcus aureus, demonstrating promising photodecontamination performance.

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Organic Cation Engineering in 2D Perovskites: Unravelling the Role of MA^+ and FA^+ on Stability and Structural Evolution

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

Three-dimensional (3D) halide perovskites have emerged as an alternative photovoltaic material class, combining low-cost fabrication with tunable bandgaps and high optoelectronic performance. Their single-junction power conversion efficiencies now rival crystalline silicon, yet further efficiency gains demand tandem architectures. In perovskite-silicon tandems, the wide-bandgap (WBG) top cell typically employs mixed-halide 3D perovskites, which suffer light-induced phase segregation into iodide- and bromide-rich domains. This segregation generates point defects, such as vacancies, interstitials and antisites, that can act as non-radiative recombination centres, undermining open-circuit voltage, reducing overall efficiency and compromising long-term stability.
Two-dimensional (2D) perovskites offer an elegant solution. Their single-halide composition inherently resists light-driven segregation, while bulky hydrophobic spacer cations bolster moisture resilience. Moreover, the natural quantum-well structure of 2D layers enhances exciton confinement and imparts superior structural stability, addressing the principal limitations of their 3D counterparts.

In this presentation, I will discuss the role of methylammonium (MA^+) and formamidinium (FA^+) cations in influencing the structure and stability of 2D perovskite films. Leveraging Atomic Force Microscopy (AFM) and X-ray Diffraction (XRD), we evaluate MA- and FA-based organic structures to highlight variations in film morphology, crystallinity, and stability. These insights offer practical direction for selecting the most suitable organic ammonium cation in 2D perovskite solar cells, contributing to the advancement of long-term device stability under operational conditions.

Assessment of Solar Energy Potential and Forecasting Accuracy in a Maritime Temperate Climate: A Case Study of Stoke-on-Trent, UK

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Lunch and Poster Session, July 1, 2025, 13:10 - 14:00

This study presents a comprehensive performance evaluation of solar energy potential in Stoke-on-Trent, UK, using high-resolution meteorological and solar irradiance data acquired from Solcast, spanning 2021-2024. The investigation examines Global Horizontal Irradiance (GHI) and Direct Normal Irradiance (DNI) patterns to determine solar power feasibility within this maritime temperate region. Temporal analysis across daily, monthly, and seasonal timeframes reveals characteristic solar resource distributions, showing summer irradiance peaks of 800 W/m^2 contrasting with winter lows of 300 W/m^2. The study implements various machine learning techniques for solar irradiance prediction, evaluating Decision Trees, Support Vector Machines (SVM), Random Forest, and Naïve Bayes approaches. Analysis shows Naïve Bayes and SVM algorithms achieving superior classification accuracy at 72%, with SVM demonstrating marginally better results across precision, recall, and F1-score measurements. The research confirms substantial solar generation potential in Stoke-on-Trent despite its northerly position, particularly during summer periods when daylight persists from 5:30 AM until 8:30 PM. However, marked seasonal fluctuations highlight the importance of optimized system design and potential storage integration for consistent year-round power delivery. This study enhances knowledge of solar resource assessment within medium-sized British urban areas while establishing an analytical framework applicable to comparable temperate climate zones.

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