AMBER

A World Leading SFI Research Centre

Science Foundation Ireland For what's next

Advancing——Materials for Impact

Internal Conference 2024
Programme & Book of Abstracts

ambercentre.ie
@ambercentre

HOST INSTITUTION

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

PARTNER INSTITUTIONS

CRANN, RCSI, UCC, Tyndall, DCU, University of Limerick, TUS, University College Dublin

FUNDED BY:

Science Foundation Ireland For what's next

Welcome to the AMBER Conference 2024!

Conference Structure

The intent of the conference is to review progress on our scientific programmes across our four research themes of ICT, Energy, Health, and Sustainable Functional Materials. The format will be a mixture of talks and poster sessions. To encourage cross centre collaboration and engagement, we are making these abstracts available to all participants in advance of the conference.

For each of the thematic areas the Theme Leads have selected 4 abstracts from the submissions to be presented at the meeting in the form of a 7min talk with 3mins of questions, those selected to give a talk have been contacted. All other abstract submissions will be presented as a poster at the poster sessions. In keeping with our sustainability goals we'd encourage you to reuse a poster prepared in the last year or so. A full conference agenda can be found below.

NEW: Post-Doc & PhD Researcher Collaboration Session

Structure: Following feedback from researchers regarding last year's conference, at this year's conference there will be a 45-minute Collaboration Session at 11:10 am on the morning of Day 1. Researchers are encouraged to network with a focus on collaborating across disciplines and institutions to pitch a project that focuses on the AMBER themes of ICT, Engineered Functional Materials/Sustainable Materials, Energy and Health.

Judging: The group project pitch must be submitted online via an application form which will be shared at the conference by the end of Day 2 – 2pm on Tuesday 16th April 2024. Judges from AMBER will shortlist the projects in the following weeks and inform those who are through to the next round. Those project teams will then be invited to pitch their project to the AMBER Executive on 23rd April and a final round of judging will follow with the winning project team informed the following day.

Prize: There is a prize of €5,000 available for the winning project and team to facilitate materials, national travel and access to infrastructure to develop their project.

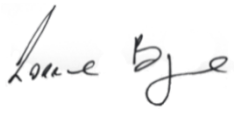
Conference Workshops

There will also be a series of workshops on Day 2 focused on training and cross Centre engagement, the topics for the workshops are chosen by researchers from across the Centre.

Image Competition

AMBER Conference attendees were invited to enter the image competition which is an opportunity to display images of your research work from the past 12 months. Images entered into the competition will be showcased during the conference and prizes will be given on the evening of Monday 15th April at the Conference.

We look forward to seeing you at the conference,



Prof. Michael Morris, Director AMBER ***Dr. Lorraine Byrne, Executive Director AMBER***

Contents

Agenda

DAY 1 - Monday 15th April 2024

Start	Finish	Duration	Item / Speaker	
10:00	10:30	00:30	Conference Registration & Refreshments	
10:30	10:50	00:20	Open Address: Dr Ciaran Seoighe, Deputy Director, SFI	
10:50	11:10	00:20	Guest Speaker: Laura H. Lewis Distinguished University & Cabot Professor, Chemical Engineering Distinguished University & Cabot Professor, Mechanical & Industrial Engineering, Northeastern University	
11:10	11:55	00:45	Post-Doc & PhD Collaboration Session	
12:00	12:15	00:15	**Theme Parallel Session 1 - Materials for ICT** Theme research highlights since last meeting	**Theme Parallel Session 1 - Materials for Health** Theme research highlights since last meeting
12:15	12.25	00:10	**Cansu Ilhan** 'Modulating Transition Metal Dichalcogenides properties through introducing impurities'	**Sinead O'Rourke** 'Check your sources: investigating the impact of tissue source in the immune response to ECM-derived biomaterials'
12.25	12.35	00:10	**Simon Lenne** 'Separation of spin-orbit torque and thermal effects in Mn2RuGa'	**Tugdual Haffner** 'Nerve-derived Tissue Matrix Bioink Concentration Influences Neurite Outgrowth and Substrate Alignment of 3D Printed Conduits'
12.35	12.45	00:10	**Dr Hodjat Hajian** 'A reprogrammable metasurface for LiDAR applications'	**Roisin Lynch** 'Regulation of anti-inflammatory immune responses by PLGA particles is dependent on particle size and the alpa v beta 3 integrin mechanosensor'
12.45	12.55	00:10	**Dr Farzan Gity** 'What if the continuous large-area grown	**Juan Carlos Palomeque** 'Development of microRNA-155-functionalised collagen-based scaffolds for anti-inflammatory and

			"monolayer" 2D material film is not just monolayer?'	pro-angiogenic outcomes in wound healing'
13:15	14:30	01:15	**Lunch**	
14:30	14:50	00:20	Guest Speaker: Jos Malda Professor: Veterinary Medicine, Department Clinical Sciences, Equine sciences Equine Musculoskeletal Biology Utrecht University	
14:50	15:50	01:00	**Poster Session 1** ICT and Health (2X 30 min sessions with half of presenters presenting in each)	
15:50	16:05	00:15	**Break**	
16:05	16:20	00:15	**Theme Parallel Session 2 - Materials for Energy** Theme research highlights since last meeting	**Theme Parallel Session 2 - Sustainable & Functional Materials** Theme research highlights since last meeting
16:20	16:30	00:10	**Anna Ciotti** 'Computational investigation of nitrate electroreduction on Cu, Zn and Zn93Cu7 metal catalysts'	**Vanja Juric** 'Yeast surface codisplay of PETase, MHETase and hydrophobin as a whole-cell biocatalyst for the degradation of PET'
16:30	16:40	00:10	**Dr Daniele Douglas Henry** 'The collaborative use of Electron Microscopy and Density Functional Theory for the characterization of exfoliated two-dimensional PtSe2 nanoflakes.'	**Dr Shardul Mukim** 'The presence of disorder is ubiquitous in the manufacturing of graphene and graphene nanodevices.'
16:40	16:50	00:10	**Rebecca Forde** 'Marine Waste Derived Carbon Materials for use as Sulfur Hosts for Lithium-Sulfur Batteries'	**Dr Saranya Rameshkumar** 'Functionalised electrospun nanofibrous membranes for selective separation applications'
16:50	17:00	00:10	**Jonathan Elliot** 'Optimisation of conjugate heat transfer in liquid	**Muireann Cosgrave** 'Synthesis of novel materials for printing and film formation

			cooled heat sinks with localised heat sources'	Diblock Polypeptide Hydrogels as Bioinks for 3D Printing in Tissue Engineering'
17:10	18:10	01:00	**Poster session 2** - Energy & Sustainable/Functional Materials (2X 30 min sessions with half of presenters presenting in each)	
18:10	18:45		**Drinks Reception**	
18:45			**Awards & Dinner**	

DAY 2 - Tuesday 16th April 2024

Start	Finish	Duration	Item / Speaker
09:30	10:00	00:30	Tea & Coffee
10:00	11:00	01:00	Workshop 1 – EPE & RTE Brainstorm
11:00	11:10	00:10	**Break**
11:10	11:55	00:45	Workshop 2 – Early career in research & how to get published (Panel)
11:55	12:05	00:10	**Break**
12:05	12:45	00:45	Workshop 3 – Commercialisation (Panel)
12:45	13:45	01:00	**Lunch**
13:45	16:15	02:30	CRANN & AMBER Ops Strategy Session (Separate Invitation)

Materials for Energy

2.1 Title: Computational investigation of nitrate electroreduction on Cu, Zn and Zn93Cu7 metal catalysts (Talk)

Authors: Anna Ciotti, Johnathan Sharp, Hayley Andrews, Shaktiswaran R. Udayasurian, Tengfei Li, Max García-Melchor

Affiliation: Trinity College Dublin

Abstract: Due to their high water solubility, nitrates are an ubiquitous pollutant in groundwaters, which endanger both human health and the environment. Thus, research is focusing on developing electrocatalysts to convert them into useful chemical.

In this scenario, I will present our findings on the nitrate reduction to NH2OH on Cu, Zn and Zn93Cu7 catalysts, to synthesize cyclohexanone-oxime. Coherently with the experiments carried out by the group of Dr. Li, we found N2 evolution to be mostly favoured on Zn. Furthermore, we assessed the energetics of *NH2OH desorption, which would lead to oxime formation, and of its hydrogenation to NH3. On Cu, the energy landscape was in agreement with the selectivity towards NH3 observed experimentally, while on Zn the high barrier for *NH2OH hydrogenation was found to advantage its desorption. The Zn93Cu7 alloy instead displayed the lowest barrier for *NH2OH hydrogenation and an exergonic *NH2OH desorption, coherently with the enhanced oxime and NH3 production of Zn93Cu7 with respect to the parent metals.

2.2 Title: "The collaborative use of Electron Microscopy and Density Functional Theory for the characterization of exfoliated two-dimensional PtSe2 nanoflakes. (Talk)

Authors: Danielle Douglas-Henry, Ilias M. Oikonomou, Thomas Brumme, Zdenek Sofer, Thomas Heine and Valeria Nicolosi

Affiliation: Trinity College Dublin

Abstract: Transition Metal Dichalcogenides (TMDs) are a class of layered van de Waals materials that consist of a transition metal (M) and chalcogen (X2) with a chemical formula MX2[1]. These materials have gleaned much popularity due to their wide range of bandgaps [2] and the variety of applications they are suited for [3]. Platinum Diselenide (PtSe2), in particular, has shown promise with its high room-temperature mobility, strong layer-dependent band structure and high stability in the air [4,5].

In this study, structural characterization and comparative modelling of few-layer exfoliated PtSe2 nanosheets was done by combining Scanning Transmission Electron Microscopy (STEM) and Density Functional Theory (DFT) simulations. The defects induced through liquid phase and mechanical exfoliation were studied and compared. Low voltage imaging was utilized to image

point defects present. The effect of point defects on the electronic structure is modelled using ab-initio DFT calculations.

[1] K. S. Novoselov et al., Science, vol. 353, no. 6298, (2016).
[2] A. Chaves et al., npj 2D Mater Appl, vol. 4, 29, (2020).
[3] S. Manzeli et al., Nat Rev Mater, vol. 2, 17033, (2017).
[4] Y. Gong et al., Nano-Micro Letters, vol. 12, no. 1, (2020).
[5] G. Wang et al., Advanced Materials, vol. 33, no. 1, (2021).

2.3 Title: Marine Waste Derived Carbon Materials for use as Sulfur Hosts for Lithium-Sulfur Batteries (Talk)

Authors: Forde, Rebecca; Brandão, Ana Teresa; Bowman, Deaglán; State, Sabrina; Costa, Renata; Enache, Laura-Bianca; Enachescu, Marius; Pereira, Carlos; Ryan, Kevin; Geaney, Hugh; McNulty, David

Affiliation: University of Limerick

Abstract: Lithium-sulfur (Li-S) batteries offer a promising alternative to conventional lithium-ion batteries, aiming to enhance battery technology and address resource limitations. Sulfur has advantageous properties like high specific capacity (1672 mA.h.g-1), low cost, lightweight, and abundance in the Earth's crust, presenting itself an attractive option for battery applications. Li-S systems outperform Li-ion chemistry in terms of affordability, safety, environmental impact, and gravimetric energy density. Despite their potential, practical implementation faces obstacles such, as sulfurs insulating nature, volume expansion, and the polysulfide 'shuttle' effect. To overcome these challenges, sustainable carbon hosts have garnered interest in aims to mitigate these effects. In this study, blue shark gelatine and prawn chitins (from seafood waste) were prepared via a one-step carbonisation process to obtain porous carbon materials. These biomass derived carbons were then used as sulfur hosts for use in cathodes for Li-S batteries, that exhibited high specific capacities, reversable cycling and long cycle life.

2.4 Title: Optimisation of conjugate heat transfer in liquid cooled heat sinks with localised heat sources (Talk)

Authors: Jonathan Elliott, Prof. Anthony Robinson

Affiliation: Trinity College Dublin

Abstract: As technology advances, the overall power density requirements of integrated circuit packages are rapidly increasing. However, thermal management technology has not developed at anywhere near the same rate. This has led to a technological disparity between advanced electronics and associated cooling technologies, as well as giving rise to thermal bottlenecks which limit overall performance and hinders the advancement of electronic devices and systems.

The present research aims to engineer advanced convective cooling and heat spreading technology by gaining a deeper understanding of the conjugate heat transfer problem, with subsequent implementation of lightweight and low-cost polymers together with state-of-the-art heat spreading material. The multiphysics conjugate problem will be addressed by developing new design methodologies which leverage multi-objective optimisation to inform both the thermal-fluids design and materials selection, creating the opportunity to tailor the cooling system design to specific applications. By prioritising the minimisation of multiple parameters such as the hydraulic penalty and device junction temperature, the goal is to develop an automated optimisation and materials selection process with rapid design cycle times that can keep pace with the rapidly evolving demands of the electronics industry.

2.5 Title: Thermokinetic insights of functionalized hemicellulose structural motifs (Poster)

Authors: Leandro Ayarde-Henríquez, Jacopo Lupi, Bernardo Ballotta, Stephen Dooley

Affiliation: Trinity College Dublin

Abstract: This study assesses the thermodynamic and kinetic effects of functional groups on the pyrolytic depolymerization of β-D-xylopyranose, a pivotal hemicellulose motif. Two distinct moieties, namely, 2-O-acetyl-β-D-xylopyranose and 4-methoxy-5-carboxy-β-D-xylopyranose, have been meticulously selected to conduct this investigation as they have been experimentally isolated from hemicellulose plant matter, a biomass main component relatively less studied compared to cellulose.

Through state-of-the-art density functional and transition state theory, we have calculated critical thermochemical data to develop reliable kinetic models. The close agreement (< 0.5 kcal mol^{-1}) between computed and experimental enthalpies of formation for pyrolytic products evidence the robustness of our methodology. The ring-opening barrier falls approximately within 43.8-47.5 kcal mol^{-1}, whereas ring-contraction and elimination exhibited comparable activation enthalpies ranging from 61.0 to 81.1 kcal mol^{-1}. The thermochemical and kinetic analyses showed that substituents lower the barrier by 1.9-8.3 kcal mol^{-1} and increase the rate constant by a factor ranging from 0 to 104.

2.6 Title: Bismuth and Silicon Alloying Anodes for High-Energy-Density Potassium-Ion Batteries (Poster)

Authors: Kwadwo Asare Owusu and Kevin M. Ryan

Affiliation: University of Limerick

Abstract: Energy storage devices (ESDs) are crucial for integrating renewable energy sources and reducing reliance on fossil fuels. Lithium-ion batteries (LIBs) dominate the market, but their high cost and limited supply challenge long-term sustainability. Potassium-ion batteries (PIBs) offer promise due to lower costs and abundant resources. However, practical PIBs with high energy

density and long cycle life remain elusive. This study investigates bismuth (Bi) and silicon (Si) as robust PIB anode materials. Unlike carbonaceous materials, Bi and Si offer higher capacitances. Si, with its high theoretical capacity, exhibits a promising potential of 995 mAh/g. Bi presents a stable K3Bi phase with a theoretical capacity of 385 mAh/g. This research advances the understanding of Bi and Si as viable anode materials for PIBs, contributing to sustainable energy storage solutions.

2.7 Title: CO2 Loss into Solution: An Experimental Investigation of CO2 Electrolysis with a Membrane Electrode Assembly Cell (Poster)

Authors: Weiming Liu, Harry Dunne, Bernardo Ballotta, Allyssa A Massie, Mohammad R. Ghaani, Kim McKelvey, Stephen Dooley

Affiliation: Trinity College Dublin

Abstract: In pursuit of commercial viability for CO2 electrolysis, this study investigates the operational challenges associated with Membrane Electrode Assembly (MEA)-type CO2 electrolysers, with a focus on CO2 loss into the solution through HCO3-/CO32- ion formation. Utilizing a silver electrode known for selectively facilitating CO2 to CO conversion, the interaction between CO2 loss and OH- ions at varying current densities was carefully examined. At lower current densities, it was revealed that CO2 loss, predominantly in the form of HCO3-/CO32-, significantly reduces the efficiency and durability of the CO2 reduction process. Conversely, at higher current densities, CO2 loss plateaus during the Hydrogen Evolution Reaction under a CO2 atmosphere, suggesting that electrolyte-induced cathode flooding limits the access of CO2 to the electrode sites. This flooding accelerates the precipitation of (bi)carbonate salts, further impacting the lifespan of the electrolyser negatively. Through continuous monitoring of electrolyte pH changes and carbon balance analysis, insights into the mechanisms of (bi)carbonate ion formation and salt precipitation are provided, offering directions for future research aimed at developing more efficient and durable Electrochemical CO2 Reduction Reaction systems.

Keywords: Membrane Electrode Assembly cell, CO2−OH− neutralization, Electrochemical CO2 Reduction Reaction (ECO2RR), Hydrogen Evolution Reaction (HER)."

2.8 Title: "A solvent-based novel process for pharmaceutical blister layer delamination using biodegradable green solvent for recovery of metal and plastic layers (Poster)

Authors: Shital B Potdar, Mukesh Pednekar, Maria Tierney, Ramesh Babu Padamati
Affiliation: Trinity College Dublin
Ramesh Babu Padamati Email: babup@tcd.ie

Abstract: Pharmaceutical blister packs comprise multiple layers, consisting of polymers and aluminium, to create a protective barrier against degradation. Blister packaging is better suited

for solid medications compared to bottles, as it helps prevent rapid deterioration, especially with frequent use.

Due to the multi-material structure of pharmaceutical blister packages, the discarded packages are typically landfilled or incinerated, although when separated, both metallic and polymeric fractions would be recyclable. The present work proposes a novel process for separating aluminium and polymers from pharmaceutical blister waste using a solvent-based technology. The delamination of polymers aluminium and recovery of inks from blisters is confirmed by FTIR, DSC, and TGA analysis, and visual inspection of the delaminated blister layers recovered. The delaminated polymer and aluminium layers can be separated using a technique such as electrostatic separation, and recovered layers can be recycled. Also, the work demonstrates the recyclability of the solvent used in the blister delamination process, making the whole process circular and sustainable.

2.9 Title: Low-dimensional SnSe – Ti3C2 MXene Composite as Binder-free Anode for Energy Storage Applications (Poster)

Authors: Kavin Arunasalam, Jesus Medina Santos, Meiying Liang, Teng Zhang, Prof. Yury Gogotsi and Prof. Valeria Nicolosi
Affiliation: Trinity College Dublin

Abstract: Two-dimensional (2D) materials exhibit unique structural and electronic properties such as reduced thickness, high conductivity, packing density and tuneable band gap.[1] These properties present compelling opportunities for their applications in sustainable battery technologies.[1] Sodium-ion batteries (SIBs) are attracting great interest as an alternative to lithium-ion batteries due to their material abundance, lower cost, and environmental sustainability. However, the quest for a high-performance anode for SIBs remains challenging owing to the severe volume expansion caused by the intercalation of the large Na-ion.

Tin (II) selenide (SnSe), a layered 2D material, demonstrates very high theoretical capacity as an anode for sodium and lithium-ion batteries. Nevertheless, its instability primarily, attributed to the substantial pulverization of active materials during cycling, poses a challenge.[2] To address this, we investigated a novel 2D composite material comprising SnSe nanoparticles and MXene (Ti3C2Tx) nanosheets to be used as an anode in batteries. Due to the exceptional conductivity and viscosity of MXene [3], it can act as a conductive binder in this composite eliminating the need for traditional non-conductive binders like PVDF and CMC. This reduces the dead volume in the electrode and enhances its specific capacity. Additionally, the MXene layers with terminating fluorine functionals promote the growth of stable solid-electrolyte interfaces (SEI) improving the overall Coulombic efficiency of the battery.[4] Further optimization studies were done with VC and FEC electrolyte additives. Characterization techniques, including XPS, SEM, EDX, XRD, and AFM were performed on the composite nanomaterial to study its morphology, as well as compositional and structural changes upon processing. The electrode material showed a high initial discharge capacity of 700 mAh/g and 98% Coulombic efficiency for 100 cycles in lithium-

ion batteries. This shows promise in overcoming the instability issues of SnSe, thereby improving the performance and longevity of SIBs for sustainable energy storage solutions.

References

[1] Jie Wang, et al., Nature Communications, 2021, Vol. 12
[2] Wei Wang, et al., Small, 2017, Vol.13
[3] Mohamed Alhabeb, et al., Chemistry of Materials, 2017 Vol. 29
[4] Yuantao Tan, et al., ACS Applied Materials & Interfaces, 2020, Vol. 12

2.10 Title: "Electrochemical behaviour of chemically treated conductive polylactic acid current collectors in additively manufactured (3D-Printed) symmetric carbon supercapacitors. (Poster)

Authors: Matthew Ferguson, Vladimir Egorov, Yan Zhang, Umair Gulzar, Colm O'Dwyer
Affiliation: University College Cork

Abstract: Producing reliable, long-lasting, and efficient energy storage devices to meet the growing energy needs of the world remains a foremost research goal in materials science. 3D-printing (also known as Additive Manufacturing) provides many benefits to this research [1-8], allowing for excellent customization and freedom of design, while eliminating waste material in the manufacturing process. Wearable electronics, medical implants, and the Internet of Things will doubtless benefit from the advantages provided by additive manufacturing.

Our previous studies compared the electrochemical performances of symmetric carbon-based supercapacitor devices made using two 3D-printing techniques, SLA (stereolithography) and FDM (fused deposition modelling). Though possessing excellent cycle life, the conductive polylactic acid (PLA) FDM printed current collectors suffered from high resistance and poor cyclic voltammetry curves (far from the rectangular shape of ideal electronic double-layer capacitors). This study aims to improve the conductivity of the FDM current collectors via chemically induced surface modification [9]. Both dimethylformamide (DMF) and aqueous potassium hydroxide (KOH) treatments are used for this purpose. The untreated, DMF-treated, and KOH-treated FDM current collectors are loaded with 1:1 by mass single-walled carbon nanotubes and graphene nanoplatelets carbon slurry, placed within stereolithography (SLA) 3D-printed casings, and assembled as supercapacitor cells (separated by glass microfiber filter separators soaked in 6 M aqueous KOH electrolyte).

Results obtained at the time of writing indicate that the DMF treatment method used in this study results in little change in electrochemical performance compared to the untreated FDM current collector cells. The KOH treatment method has proven to be more effective at increasing the conductivity of the FDM current collectors. A tenfold decrease in the FDM current collector resistance is measured, which correlates with the improved (yet still far from ideal) cyclic voltammetry response for these EDLC supercapacitors. However, galvanostatic charge-discharge tests reveal that the benefits of the KOH-treatment come at a cost of worsened cycling stability and rate capability response. Further investigations into these treatment methods could

determine an ideal middle ground to maximise the benefits to the current collectors, while minimising the adverse effects of the treatments.

References

[1] A. Ambrosi and M. Pumera, ""3D-printing technologies for electrochemical applications.,"" Chemical society reviews, vol. 45, no. 10, pp. 2740-2755, 2016.
[2] V. Egorov and C. O'Dwyer, ""Architected porous metals in electrochemical energy storage.,"" Current Opinion in Electrochemistry, vol. 21, pp. 201-208, 2020.
[3] V. Egorov, U. Gulzar, Y. Zhang, S. Breen and C. O'Dwyer, ""Evolution of 3D printing methods and materials for electrochemical energy storage.,"" Advanced Materials, vol. 32, no. 29, p. 2000556, 2020.
[4] U. Gulzar, C. Glynn and C. O'Dwyer, ""Additive manufacturing for energy storage: Methods, designs and material selection for customizable 3D printed batteries and supercapacitors.,"" Current Opinion in Electrochemistry, vol. 20, pp. 46-53, 2020.
[5] J. Li, M. Leu, R. Panat and J. Park, ""A hybrid three-dimensionally structured electrode for lithium-ion batteries via 3D printing.,"" Materials & Design, vol. 119, pp. 417-424, 2017.
[6] A. Maurel, M. Courty, B. Fleutot, H. Tortajada, K. Pdrashantha, M. Armand, S. Grugeon, S. Panier and L. Dupont, ""Highly loaded graphite–polylactic acid composite-based filaments for lithium-ion battery three-dimensional printing.,"" Chemistry of Materials, vol. 30, no. 21, pp. 7484-7493, 2018.
[7] S. O'Hanlon and C. O'Dwyer, ""Electrodeposition onto Conductive Additive-Impregnated 3D Printed Polylactic Acid Electrodes.,"" Journal of The Electrochemical Society, vol. 169, no. 8, p. 082514, 2022.
[8] B. Yao, S. Chandrasekaran, J. Zhang, W. Xiao, F. Qian, C. Zhu, E. Duoss, C. Spadaccini, M. Worsley and Y. Li, ""Efficient 3D printed pseudocapacitive electrodes with ultrahigh MnO2 loading.,"" Joule, vol. 3, no. 2, pp. 459-470, 2019.
[9] S. Srinivasan K. V, J. Santo and P. Penumakala, ""Effect of surface modification of printed electrodes on the performance of supercapacitors,"" Journal of Energy Storage, vol. 56, no. B, p. 106043, 2022.

2.11 Title: Lignin-derived materials for sustainable development of ionic thermoelectric supercapacitors (Poster)

Authors: Muhammad Muddasar, Mario Culebras, and Maurice Collins
Affiliation: University of Limerick, Limerick

Abstract: The growing demand for eco-friendly alternatives has driven research into sustainable materials. Lignin, a waste product from the paper and pulp industry, has emerged as a promising option for advanced energy applications. This study examines lignin as a potential material for the synthesis of ionic thermoelectric membranes and carbon-based materials. Ionic membranes were designed with hierarchically aligned channels, resulting in a remarkable Seebeck coefficient of 5.71 mV/K under axial temperature gradient. Furthermore, lignin-based porous carbon materials were synthesized using a template-free tailoring technique. These materials exhibit exceptional performance as supercapacitor electrodes, with a superior specific capacitance of 102.3 F/g at 0.5 A/g and retains 70.3% capacitance at 20 A/g. The integration of lignin-based membranes and porous carbon electrodes offers a promising avenue for developing lignin-derived ionic thermoelectric supercapacitors, enabling simultaneous energy harvesting and storage, while contributing to waste utilization and sustainable materials for environmentally friendly energy production and storage solutions.

2.12 Title: Nanowood-based thermoelectric material and its application for waste heat recovery. (Poster)

Authors: Ievgen Nedrygailov, Scott Monaghan, Paul Hurley and Justin D. Holmes
Affiliation: University College Cork

Abstract: The energy transition, that is, the transition from fossil fuels to renewable energy sources, is among the most important challenges of modern science. One part of the energy transition is the use of waste heat as an energy source to generate clean electricity, which could be achieved using thermoelectric generators based on ionic materials. In this presentation, we discuss the prospects for the production and use of a new ionic thermoelectric material - nanowood. The technology for producing nanowood is described, as well as the prospects for its practical use in ionic thermoelectric supercapacitors.

2.13 Title: Novel Technique for Developing E-Textiles: Printing MXene Supercapacitors on Fabrics for Wearable Electronics (Poster)

Authors: Anastasiia Shandra, Ke Li, Dahnan Spurling, Oskar Ronan, Valeria Nicolosi
Affiliation: Trinity College Dublin

Abstract: The escalating demand for miniaturized, flexible wearable electronics propels the rapid growth in the field of e-textiles. As e-textiles necessitate energy storage solutions that are not only compact but also conformable, microsupercapacitors emerge as an attractive option due to their exceptional power density and prolonged operational lifespan. Leveraging textile properties like flexibility, breathability, and strength, we present an innovative method for fabricating e-textiles using aerosol-jet printing (AJP) with Ti3C2Tx MXene inks. AJP offers high resolution and cost-effectiveness for rapid prototyping, while Ti3C2Tx MXenes exhibit excellent electrical conductivity, mechanical flexibility, and facile processability in stable, viscous, aqueous, additive-free colloidal suspensions.

Through systematic exploration on cotton, polycotton, and polyester, we achieve flexible electrodes with remarkable capacitance (up to 540 mF cm-2 with 10 layers) with exceptional high-rate performance, capacitance retention, minimal equivalent series resistance, and outstanding cycling stability. These electrodes also maintain their performance after rigorous washability testing. Optimized microsupercapacitors on cotton exhibit impressive capacitance (up to 381 mF cm−2) when coupled with a poly(vinyl alcohol)/sulfuric acid gel electrolyte, surpassing existing printed MXene/textile-based microsupercapacitors.

2.14 Title: Data-driven Magnetic Materials Inverse Design (Poster)

Authors: Matteo Cobelli, Luke Gilligan, Michelangelo Domina, Stefano Sanvito
Affiliation: Trinity College Dublin

Abstract: Magnetic materials have diverse applications across multiple sectors, ranging from electric motors to sensors, and wind turbines just to name a few. The demand for novel magnetic

materials, tailored for specific applications, is higher than ever. However, the recent advances in technology have not been matched by a comparable rate of material discovery, largely due to the unavoidable low throughput of experimental synthesis. For these reasons, there is a growing need for alternative approaches to material discovery, potentially involving in-silico predictions. In this work, we present a data-driven approach to the design of magnetic materials. We address various challenges that afflict the material-discovery pipelines, for which we find solutions that leverage recent advancements in artificial intelligence. The result is an end-to-end workflow for materials inverse-design with a strong interdisciplinary nature, borrowing techniques from various domains of machine learning, ranging from statistical modelling to natural language processing.

2.15 Title: Increasing efficiency and longevity of solar PV systems through enhanced passive convection (Poster)

Authors: Erik Soderholm, David McCloskey
Affiliation: Trinity College Dublin

Abstract: Silicon solar cells are reaching the limits of efficiency and other ways to increase output will be needed. Based on the amount of uptake when PV systems reach end of life there could be a significant recycling / e-waste issue. Cost effective methods to prolong lifetime could be hugely beneficial towards solving this problem. Reducing the negative thermal effects on solar PV systems by reducing operating temperatures can increase the longevity and efficiency of these systems. This is a achieved through passive heat sinking specifically designed for the large area of a solar panel.

2.16 Title: Extension of Chemical Reaction Networks and Refinement of Kinetic Parameters through Computational Strategies for Electrochemical CO2 Reduction Cells (Poster)

Authors: Bernardo Ballotta and Stephen Dooley
Affiliation: Trinity College Dublin

Abstract: The electrochemical reduction of CO2 is a process that has attracted considerable attention from the scientific community due to the significant role it would have in the reconversion and lowering of the CO2 concentrations in the atmosphere. In the last years, numerous experimental and computational studies have been carried out with the aim of improving the efficiency of CO2 reduction reactors, and our understanding of the chemical reaction mechanisms that govern its functioning. So-called 'digital twins', i.e. computational models based on multiphysics simulations capable of representing complex systems such as electrochemical reduction cells, are enjoying considerable relevance. However, the parameters used as input data in such simulations may have been determined through experimental or computational techniques that do not fully represent the chemical-physical conditions of the system. The results obtained from these simulations demonstrate a poor reproducibility of the experimental results, and a poor fidelity to reasonable estimations of physical quantities. Regarding the chemical reaction mechanism, authors of recently published works select a limited number of reactions that can occur in solution or on the surface of electrodes, very often

simplifying multistep processes into a single step. These simplifications define a strong deviation of a physically real description. In recent review articles on this topic, it has been highlighted that kinetic parameters regarding chemical reactivity in solution and on surfaces used in such models have been poorly determined, yet no complete or detailed assessment is present in the literature. In this work, we discuss what is necessary to describe the CO2 reduction reaction mechanism fundamentally, in both aqueous solution and catalytic surface phases, also including solvation. A comprehensive survey of literature knowledge is presented. Subsequently, methodologies are proposed to accurately determine the molecular thermodynamic and reaction kinetic parameters based on quantum mechanics (QM) and molecular dynamics (MD) simulations. Improving these parameters and creating more detailed computational models for multidimensional multiphysics simulations would allow experimental data to be reproduced not only qualitatively but also quantitatively, and experimental cell designs to be virtually analyzed to increase operational efficiency,and our understanding of the CO2 reduction phenomena.

2.17 Title: Advancing Energy Planning Through Integrating Stochastic Analysis with EnergyPLAN tool: StEP Model (Poster)

Authors: Seyed Mohammad Shojaei, Reihaneh Aghamolaei, Mohammad Reza Ghaani
Affiliation: Trinity College Dublin

Abstract: This research introduces StEP (Stochastic EnergyPLAN), a novel framework that integrates Monte Carlo simulations with EnergyPLAN software, to address its limitations of deterministic modelling approach. Addressing uncertainties in renewable resources, climate conditions, energy system components, and hourly distribution patterns, StEP enhances energy planning by reflecting real-world variability and sensitivities. It automates scenario generation and employs parallel computing to explore numerous possibilities within uncertainty bounds. This approach deepens understanding of factors affecting energy system performance, supporting the creation of effective, resilient strategies. While StEP is primarily designed for analysing and planning energy systems under uncertainty, its comprehensive analysis of variables and scenarios can indeed provide valuable inputs for multiobjective optimisation purposes as well. A case study of Trinity College Dublin's energy system, applying StEP for a scenario using CHP units and heat pumps, demonstrates its practicality. The insights gained underline its value for policymakers and stakeholders in devising adaptable, future-proof strategies.

2.18 Title: Optimizing Hydrogen Refueling Stations in Ireland for Sustainable Transport: A Cost and Component Analysis (Poster)

Authors: Colm Coegh, Mohammad Reza Ghaani

Affiliation: Trinity College Dublin

Abstract: Addressing the urgent need for decarbonizing the transport sector, this project focuses on optimizing component sizing for standalone hydrogen refueling stations in Ireland to reduce projected hydrogen costs in 2023, 2030, and 2050. By leveraging HOMER Pro for the optimization

of electrolyzers, wind turbines, photovoltaic (PV) systems, hydrogen storage tanks, and battery storage across Dublin, Galway, Belfast, Cork, and Wexford, it identifies Ireland's southern/southeastern region as most cost-effective, thanks to its high solar index and strong winds. The study found that, in 2023, PV systems were excluded due to low power output, favoring wind turbines instead. By 2030, the energy mix shifted towards a balance, with a significant tilt towards PV by 2050. A sensitivity analysis showed that a greater PV to wind turbine ratio leads to cheaper hydrogen, with a preference for hydrogen over battery storage. This research supports the feasibility of cost-effective, sustainable hydrogen fueling solutions for Ireland's transport sector evolution.

Materials for Health

3.1 Title: Check your sources: investigating the impact of tissue source in the immune response to ECM-derived biomaterials (Talk)

Authors: Sinead O'Rourke, Giovanni Gonnella, Josephine Wu, Gabriela Soares-Kronemberger, Aisling Dunne, Daniel Kelly

Affiliation: Trinity College Dublin

Abstract: Osteoarthritis (OA), is a chronic, degenerative disease, stemming from initial injuries or defects of the joint. The immune response greatly dictates disease progression and outcome for OA patients, with chronic inflammation driving further tissue degeneration and increasing need for revision surgeries following joint-replacement surgeries. As a result, modulation of the immune response has become an attractive therapeutic target to improve tissue regeneration and implant longevity in the joint, ultimately improving patient outcome.

There is now ample evidence highlighting how biomaterials can be used to modulate immune responses in vivo, steering cell phenotype from a destructive pro-inflammatory state to a more favourable pro-regenerative phenotype. The aim of this project is to investigate the immunomodulatory potential of “natural” biomaterials derived from extracellular matrix (ECM). Furthermore, to investigate whether the immune response to such biomaterials is dependent on the source of ECM used, and whether this in turn promotes tissue-specific regeneration.

3.2 Title: Nerve-derived Tissue Matrix Bioink Concentration Influences Neurite Outgrowth and Substrate Alignment of 3D Printed Conduits (Talk)

Authors: Haffner, and Buckley CT

Affiliation: Trinity College Dublin

Abstract: Peripheral nerve injury affects over one million people each year worldwide. Autografts are considered as the gold standard for nerve repair, with nerve guidance conduits (NGCs) used for small gap repairs. The overall goal of this study was to develop and characterise a new nerve-derived extracellular matrix tissue ink for biofabricating the next generation of NGCs using 3D printing.

Nerve tissue was harvested from adult porcine hind legs, solubilised, and functionalised into methacrylated nerve extracellular matrix (nECM-MA). In vitro DRG model exhibited improved neurite outgrowth for softer hydrogels reaching a maximum length with 2% nECM-MA substrates. Tissue inks consisting of different concentrations (0.5, 1, 2, 4 and 8% w/v) of material were investigated for 3D printing. Combining this tissue ink with 3D printing offers the potential to

improve mechanical properties and enhance cell behaviour driven by aligned architecture mimicking that of native nerve tissue.

3.3 Title "Size Matters; Particle size regulates the induction of anti-inflammatory responses and immune tolerance via αvβ3 mechano-sensor engagement." (Talk)

Authors: Roisin I. Lynch, Jorge Huerte-Carrasco, Ed Lavelle

Affiliation: Trinity College Dublin

Abstract: The Lavelle lab has focused on the importance of micro-biomaterial physico-chemical properties in the regulation of innate and adaptive immunity. Notably, particle size was found to be a critical factor that modulates dendritic cell activation and the subsequent polarisation of T cell responses. We have identified that biodegradable poly (lactide-co-glycolide) (PLGA) particles within the 1-2 µm diameter, drive potent secretion of IL1ra and IL-10 from key antigen presenting cells (APC's). Consequently, these anti-inflammatory APC's were proficient in priming and expanding a CD4+ regulatory T-cell (T-reg) population both in an in-vitro co-culture model and in-vivo studies.

Investigations into the mechanism behind enhanced anti-inflammatory responses revealed a key role for the integrin; αvβ3. Activation of this mechano-sensory integrin is hypothesised to be driven by changes in cell morphology and membrane tension induced by particles of the 1-2 µm range.

These findings demonstrate the therapeutic potential of biodegradable micro-particles of this size.

3.4 Title: Development of gene-activated collagen-based scaffolds for the promotion of pro-regenerative outcomes in wound healing (Talk)

Authors: Juan Carlos Palomeque Chávez, Matthew McGrath, Cian O'Connor, Marko Dobricic, Sandra Sunil, Cathal J. Kearney, Shane Browne, Fergal J. O'Brien

Affiliation: Royal College of Surgeons in Ireland

Abstract: Diabetic foot ulcers (DFUs) are chronic wounds that constitute a disabling complication of diabetes. Collagen-based scaffolds can be utilized as biomimetic templates for skin repair and may have promise for repair and remodeling of DFUs. However, DFUs present extensive gene dysregulation and such scaffolds require further functionalization to promote healing. To address this challenge we propose the gene activation of collagen-glycosaminoglycan (CG) scaffolds with microRNA-155 inhibitor (CG-anti-miR-155) which has shown anti-inflammatory and pro-angiogenic outcomes in vivo. CG-anti-miR-155 scaffolds increased the expression of anti-inflammatory (IL-10) and pro-angiogenic (VEGF) markers over 7 days post-transfection from non-

polarised (M0) macrophages. Additionally, CG-anti-miR-155 scaffolds reduced cell circularity and increased the number of CD206+ macrophages over 7 days post-transfection, indicating M2 macrophage polarisation. Taken together, this data indicates that CG-anti-miR-155 scaffolds enable the polarisation of M0 macrophages towards an M2 phenotype; key for the reduction of inflammation, promotion of angiogenesis, and the resolution of chronic wounds.

3.5 Title: Controlling Aerosol Jet printed MXene flake morphology for neural interfaces and energy storage applications (Poster)

Authors: Javier Gutierrez-Gonzalez, Dahnan Spurling, Cian O'Connor, Tara McGuire, Ke Li, Ian Woods, Adrian Dervan, Fergal J. O'Brien 3nd Valeria Nicolosi

Affiliation: Royal College of Surgeons in Ireland

Abstract: MXenes are 2D layered nanomaterials consisting of carbides and nitrides of transition metals that show excellent electrical conductivity, charge storage and biocompatibility. While typically used as aligned flakes, MXenes (Ti3C2Tx) can also fold forming a crumpled 3D structure, which hold untapped potential, harbouring properties that remain largely unexplored due to the complexity of existing methods or additional processing steps. To overcome these obstacles, this study has focused in developing a method to precisely control MXene flake morphology through 3D printing at micron-level resolution, leveraging Aerosol Jet printing (AJP) technology to explore the use of both aligned and crumpled MXene morphologies. After a systematic analysis of the printing parameters and the development of a novel monitoring system for identifying the flake morphology, this method demonstrates promising potential in the development of neural interfaces with a modulated foreign body response, and also porous all-MXene micro-supercapacitors with enhanced energy storage.

3.6 Title: Growth factor patterning into fusing microtissues: 3D bioprinting of spatiotemporal cues for cell spheroid and organoid based tissue engineering (Poster)

Authors: Josephine Y Wu, Daniel J Kelly

Affiliation: Trinity College Dublin

Abstract: Sacrificial writing into functional tissue (SWIFT) is an approach to vascularize highly cellular tissues by bioprinting sacrificial channels into an organoid-based support bath. We hypothesized we could similarly pattern spatiotemporal cues mimicking physiological development into a living matrix of cell spheroids to promote native-like tissue organization. We assembled immature, rather than pre-differentiated cell spheroids, to avoid boundary protein secretion around individual spheroids which after several days would inhibit fusion with neighboring bodies and thus fusion into larger, cohesive tissues. Using cartilage for proof-of-principle, our bioprinting support baths consisted of 2-day-old, bone marrow mesenchymal stromal cell derived chondrogenic spheroids. Transforming growth factor beta 3 (TGF-β3)

gradients drive stratified cartilage development. Therefore, we incorporated TGF-β3 into an alginate-laponite bioink with 3-week sustained delivery. Engineered tissues with only TGF-β3 released from bioprinted filaments were of superior quality to counterparts receiving standard culture medium supplementation of TGF-β3. Cartilage-bone interactions regulate development and homeostasis; thus, we developed bone morphogenetic protein 2 (BMP-2) bioinks to induce a more osteogenic phenotype in a subset of microtissues. From a bath of phenotypically homogenous spheroids maintained in a shared basal medium, we anticipate that spatiotemporally distributed growth factors via bioprinted alginate filaments can drive the formation of an osteochondral gradient. In summary, we established a platform for patterned release of growth factors alongside cell spheroid building blocks for cartilage tissue engineering and anticipate its application for delivery of various bioactive agents across diverse tissue types.

3.7 Title: Development of a progenitor loaded biomimetic scaffold for spinal cord repair applications (Poster)

Authors: Cian O'Connor, Ian Woods, Sarah McComish, Maeve Caldwell, Adrian Dervan, Fergal O'Brien

Affiliation: Royal College of Surgeons in Ireland

Abstract: Following spinal cord injury (SCI), a lesion cavity develops preventing axonal regrowth. Biomaterial scaffold implants that bridge the cavity and encourage axonal growth from neurons while delivering trophic cells may have reparative potential. By identifying the optimal neurotrophic proteins to incorporate into biomimetic biomaterial scaffolds and by tuning scaffold stiffness, we aimed to develop a novel platform that can support the delivery of trophic progenitor cells to the injured cord. Here, we show that soft biomaterial scaffolds mimicking the stiffness, protein composition and topography of the healthy cord promoted anti-inflammatory responses in supportive cord cells and enhanced neuronal growth compared to stiffer scaffolds. Furthermore, they enhanced the growth of implanted progenitor cells while also increasing the production of angiogenic, anti-inflammatory and neurogenic factors that promote neurite outgrowth from spinal cord neurons. Overall, this work outlines the development of a novel progenitor cell-loaded biomimetic scaffold platform for SCI repair applications.

Acknowledgements: This work is funded by the Irish Rugby Football Union-Charitable Trust and the Science Foundation Ireland-funded Advanced Materials and BioEngineering Research (AMBER) Centre."

3.8 Title: A Multiple-targets Inverse finite element approach for characterising multi-layered soft tissues (Poster)

Authors: Majid Akbarzadeh Khorshidi, Shirsha Bose, Brian Watschke, Evania Mareena, Caitríona Lally

Affiliation: Trinity College Dublin

Abstract: The mechanical behaviour of soft biological tissues relies on sophisticated constitutive models due to their nonlinear nature and complex microstructural compositions. Traditional curve-fitting methods may fall short in accurately characterising, especially in complex geometries. To address this, inverse finite element (FE) methods have been widely used. While loading-deformation results are sufficient for simpler models, multi-layered tissues with intricate geometries demand supplementary experimental data. This study employs a multiple-targets inverse FE approach that integrates load-bearing and boundary deformation experimental data for characterising the tissue. We aim to establish accurate tissue properties of human penile tissue, addressing the limitations of existing research in the literature and providing a more realistic understanding of penile tissue mechanics.

3.9 Title: Modulating Human Macrophage Metabolism through the Glycolytic Enzyme PKM-2 for the Generation of Regenerative Extracellular Vesicles (Poster)

Authors: Cansu Gorgun, Brenton L Cavanagh, David A. Hoey, Annie M. Curtis

Affiliation: Royal College of Surgeons in Ireland

Abstract: Pro-inflammatory (M1) and anti-inflammatory (M2) macrophages and their extracellular vesicles (EVs) play crucial roles in terms of bone regeneration. The macrophage phenotype is dependent on intracellular metabolic pathways such as glycolysis of which the enzyme Pyruvate-kinase M2 (PKM2) is involved. Therefore, we hypothesised that if we metabolically reprogram macrophages through modulation of the key glycolytic enzyme Pyruvate-kinase M2 (PKM2), we could generate EVs that were more reparative for bone repair than standard methods of macrophage EV generation. We demonstrated that activating PKM-2 in macrophages led to upregulated mRNA levels of IL10, VEGF and COX2, while significantly downregulating expression of CXCL10 and CD38, as well as IL-6 secretion. Additionally, EVs obtained from PKM-2 re-programmed human macrophages significantly enhanced tube formation in HUVECs compared to pro-inflammatory controls. These findings highlight the connection between macrophage metabolism and EV generation, suggesting the novel possibilities for therapeutically targeting macrophage metabolism to promote bone healing.

3.10 Title: The Influence of the Degenerating Nucleus Pulposus Microenvironment on Cellular Matrix Synthesis Rates (Poster)

Authors: Niamh Wilson and Conor T. Buckley

Affiliation: Trinity College Dublin

Abstract: The microenvironment of the intervertebral disc is heavily reliant on diffusion of nutrients and metabolites through the cartilage end plate and therefore varies with increasing

levels of degeneration. Degeneration of this microenvironment can impact the outcomes of regenerative therapies as it influences the function and survival of the intradiscal cells. Key microenvironmental parameters within the intervertebral disc have been previously characterised but their effect on the cellular response has yet to be elucidated. The aim of this work is to determine the effect of altering pH, glucose, and osmolarity on the matrix production rates of nucleus pulposus cells. In silico models were used to predict changes in these conditions owing to cellular consumption and production rates. Glucose consumption rates increased at higher glucose levels defining two distinct consumption rates, as reflected in the models. Future work in this area will determine the effect of varying oxygen levels on the matrix synthesis rates of intradiscal cells.

3.11 Title: Cell Penetrating Peptides for microRNA Delivery and Regulation of NP Cell Phenotype (Poster)

Authors: Marcos N. Barcellona, Tara Ní Néill, Fergal J. O'Brien, James E. Dixon, Caroline M. Curtin, Conor T. Buckley

Affiliation: Trinity College Dublin

Abstract: Low back pain is a debilitating condition primarily caused by degeneration of the intervertebral disc (IVD) and central nucleus pulposus (NP) region. Conservative and more invasive surgical interventions fail to treat the underlying degeneration, leading to explorations into driving regenerative potential of the resident NP cell population. Hence, potentially therapeutic microRNAs were investigated here, with single and paired delivery employing non-viral cell penetrating peptides (CPPs), with the aim of modulating the degenerative cascade.

In vitro studies and ex vivo organ culture in a rat model of IVD degeneration demonstrated increases in the production of glycosaminoglycans (GAGs), a key NP extracellular matrix component, following delivery of the microRNA pair 149-5p mimic + 221-3p inhibitor. A concurrent significant decrease to catabolic protein expression of MMP13 and ADAMTS5 was identified, suggesting the generation of an anti-catabolic niche whereby IVD regeneration could proceed, offering the potential of IVD cell therapeutics in the future.

3.12 Title: Penile tissue test for benchtop model (Poster)

Authors: Shirsha Bos, Majid A. Khorshidi, Evania Mareena, Caitríona Lally

Affiliation: Trinity College Dublin

Abstract: Erectile dysfunction affects 52% of men in the age range of 40 – 70 and patients not responding to conventional treatments are advised to use inflatable penile prostheses (IPPs). An IPP consists of a pair of cylinders which are placed in the corpora cavernosa (CC), a pump in the scrotal sacs and a reservoir inside the abdomen. To-date, limited mechanical characterisation has been performed on penile tissues. Understanding penile biomechanics is essential for optimising

the successful design and implantation of IPPs. The aim of this work is to accomplish this to enable more efficient IPP optimisation by developing, anatomically realistic pre-clinical testbeds with similar tissue properties matched to penile tissue need to be designed.

Whole human penile tissues was obtained and tested in compression and then segregated into individual tissues – CC, tunica albuginea (TA) and urethra for individual tissue properties. These properties was used to inform the development of the preclinical testbeds.

3.13 Title: Can X-ray-based histology be used for 3D collagen and elastin specific visualisation in vascular tissue? (Poster)

Authors: Francesco Digeronimo, Robert Johnston, Greet Kerckhofs, Brooke Tornifoglio, Caitríona Lally

Affiliation: Trinity College Dublin

Abstract: Histology currently represents the gold-standard for visualising vascular tissue microstructure. Despite allowing for the specific visualisation of tissue structural proteins, histology is a destructive technique limited to thin 2D tissue planar views. Contrast-Enhanced micro-Computed Tomography (CE-µCT) or 3D X-ray-based histology offers a non-destructive solution, providing the potential for full 3D tissue microstructural visualisation. For its optimal use in vascular tissue, however, suitable Contrast-Enhancement Staining Agents (CESAs) need to be identified which are specific to key vascular proteins, such as collagen and elastin. Phospho-Tungstic Acid (PTA) and Hafnium substituted Wells-Dawson PolyOxoMetalate (Hf-WD POM) have been suggested to preferentially bind to collagen and elastin, respectively. This study aims to investigate the binding affinity of these CESAs to collagen and elastin using vascular tissue degradation models.

3.14 Title: "Conductive melt-electrowritten MXene microfiber composite macroporous scaffolds enhance the delivery of electrical stimulation to neurons. (Poster)

Authors: Woods I, Spurling D, Sunil S, Maughan J, Gutiérrez González J, Dervan A, Nicolosi V, O'Brien F J

Affiliation: Royal College of Surgeons in Ireland

Abstract: Neurotrauma can lead to neural impairment and no regenerative therapy currently exists. Electrical stimulation(ES) shows multi-pronged pro-regenerative potential and may be enhanced by delivery through conductive biomaterials. To develop electroactive implants to facilitate ES delivery, melt-electrowritten microfiber polycaprolactone architectures of varying fiber densities (500, 750 and 1000 µm spacings) were functionalized with highly conductive MXene nanosheets (10^5S/cm) to produce implants with tunable conductivity (19.13±6.35, 14.13±2.73 and 3.03±0.46 S/cm, respectively). The conductive microfiber architectures were

then filled with a biomimetic hydrogel and freeze-dried to produce a macroporous composite scaffold. Electrical stimulation of neurons through the conductive scaffolds resulted in increased axonal length ($p<0.01$) in conductive scaffolds relative to inert ones, in a manner dependent on MXene microfiber architecture. This novel conductive microfiber scaffold has the potential act as a pro-regenerative electroactive implant for neurotrauma repair.

3.15 Title: Targeting mechanosignalling to modulate the immune response for bone repair (Poster)

Authors: Petrousek, S, Kronemberger, G S, O'Brien, G, O'Rourke S A, Shanley L, Dunne, A, Kelly, D J, Hoey, D. A

Affiliation: Trinity College Dublin

Abstract: Mechanical signals are among the most potent regulators of bone repair and may offer the potential to influence local inflammation, by acting upon the early fracture haematoma, as suggested by heightened inflammatory levels observed in mechanically unstable fractures. This study explores, for the first time, the influence of mechanics on the early immune response and subsequent bone healing outcome. This was achieved via the development of a purpose-built in vitro model replicating the local immune environment and loading conditions experienced at the bone fracture hematoma site. Using this system, we first established how local strain magnitudes can modulate macrophages, key mediators of the immune response, and further determined the impact on the later stages of vascularisation and mineralisation. We next demonstrated that local moderate strains can be utilised to direct a highly inflammatory macrophage response towards a more regenerative state, altering the vascularisation outcome. Finally, we defined a second treatment strategy, in the context of complex fractures where constrained local mechanics are particularly challenging to achieve, by modulating macrophage sensitivity to mechanical cues using newly identified mechanotherapeutics.

3.16 Title: ELECTROSTIMULATION VIA A 3D-PRINTED, BIOMIMETIC, NEUROTROPHIC, ELECTROCONDUCTIVE SCAFFOLD FOR THE PROMOTION OF AXONAL REGROWTH AFTER SPINAL CORD INJURY (Poster)

Authors: Liam M. Leahy, Ian Woods, Javier Gutierrez-Gonzalez, Jack Maughan, Cian O'Connor, Martyna Stasiewicz, Kulwinder Kaur, Michael G. Monaghan, Adrian Dervan, Fergal J. O’Brien

Affiliation: Royal College of Surgeons in Ireland

Abstract: Electrical stimulation is a promising method of promoting axonal regrowth following spinal cord injury (SCI), and its efficacy may be enhanced when applied via electroconductive scaffolds. To effectively stimulate injured axons, a novel, electroconductive scaffold for SCI repair was developed by coating 3D-printed polycaprolactone (PCL) with electroconductive polypyrrole

(PPy). The PPy layer exhibited conductivity 30 times higher than neuronal tissue. PPy/PCL scaffolds were developed as a collection of interlocking cylindrical channels, mimicking cord axonal tract structure. The scaffolds were filled with freeze-dried extracellular matrix mixture with aligned pores to further promote axonal growth. Electrostimulation delivered via this electroconductive scaffold significantly increased neurite outgrowth, highlighting this system's potential to promote axonal regrowth after SCI
This work represents the development of novel, biocompatible, electroconductive, 3D-printable scaffolds for SCI repair that can be scaled to match the native tract geometries to direct ES to promote repair after injury.

FUNDING ACKNOWLEDGEMENTS
Irish Rugby Football Union Charitable Trust, SFI AMBER Centre (SFI/12/RC/2278_P2)."

3.17 Title: Bio-fabrication of Spatially Defined Cartilage Grafts Using Microtissues Engineered in Different Oxygen Conditions (Poster)

Authors: N. Rodriguez, I. F. Goncalves, F. J. O'Brien, D. J. Kelly

Affiliation: Trinity College Dublin

Abstract: Articular cartilage (AC) is spatially organized into zones from the surface to the deep region of the tissue, each with a distinct composition and structure determining overall tissue function. Due to its avascular nature, oxygen levels in AC layers are relatively low (5-1% O2). Chondrocytes and mesenchymal stem/stromal cells (MSCs), which are often used in the regeneration of AC, are known to respond to low oxygen conditions by promoting a chondrogenic phenotype. In this study, we sought (i) to engineer phenotypically distinct cartilage microtissues (µTs) by exposing them to altered oxygen conditions (2% and 5% O2) and (ii) to use such phenotypically distinct µTs as biological building blocks in combination with melt electro-written (MEW) scaffolds to biofabricate larger, layered cartilaginous grafts. First, assessment of µT chondrogenic phenotype showed that 2% O2 significantly promotes glycosaminoglycan deposition and tends to produce more type II and less type I collagen compared to 5% O2. Then, µTs were primed for 7 days prior to fusion onto a MEW mesh. Fusion resulted in mm-scale grafts with controlled overall geometry and collagen orientation. Our findings support the combined use of low volume MEW meshes and µTs to biofabricate highly cellular grafts with superior function.

3.18 Title: Delivering Parasite-Derived Immunotherapeutics from Hyaluronic Ac-id Hydrogels Acting as Soft Tissue Supports (Poster)

Authors: Ward V, O'Dwyer J, Lalor R, Dalton J P, Duffy G P

Affiliation: University of Galway

Abstract: This research investigates hyaluronic acid hydrogels, and their role acting as soft tissue supports. To help improve material implantation, understanding the mechanical profile of the target tissue is important. This research developed a range of hydrogels suitable for subcutaneous tissue implantation and broadly tested the mechanical profiles of these materials. Another strategy to reduce the potential immune rejection from implantable materials was through the release of an immunomodulatory therapeutic. This therapy was loaded into the hydrogel with a release profile developed and optimised. The hydrogels most suitable to achieve both soft tissue support alongside drug release were used in vivo. This pilot mouse model implanted hydrogels into the subcutaneous space for 14 days. The tissue around the device was extracted at the end of the study and current work is comparing the immune response to hydrogels unloaded and therapy loaded.

3.19 Title: Biomimetic multi-layered functionalised antimicrobial scaffolds for enhanced wound healing. (Poster)

Authors: Matthew McGrath, J.C. Palomeque Chavez, Shane Browne, Fergal O'Brien

Affiliation: Royal College of Surgeons in Ireland

Abstract: Diabetic foot ulcers are a major complication for diabetic patients with a high risk of infection. In this project, a biomimetic, bi-layered antimicrobial collagen-based scaffold was developed, consisting of an epidermal, antimicrobial collagen/chitosan film to prevent wound infection and a dermal collagen-glycosaminoglycan (CG) scaffold to support angiogenesis. Biophysical properties were enhanced through 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide crosslinking, with the scaffold successfully inhibiting the growth and infiltration of staphylococcus aureus, supporting the proliferation of epidermal cells on its surface, and the proliferation of vascular cells (induced pluripotent stem cell derived endothelial cells and supporting stromal cells). Functionalisation with laminin-1 in the CG layer increased angiogenic potential, with enhanced cell coverage and vascular-tube structures seen forming throughout the scaffold. Overall, these results indicate that the bi-layered scaffold is an excellent candidate for enhancement of diabetic wound healing by preventing wound infection and supporting angiogenesis.

Acknowledgements
This work was supported by the SFI-AMBER Centre (SFI/12/RC/2278_2).

3.20 Title: Design & manufacture patient specific 3D printed stents to treat aortic coarctation (Poster)

Authors: Johnston, R D, McKenna C, O'Keeffe C, Linnane N, Bose S, Geraghty S, Kenny D, Lally C.

Affiliation: Trinity College Dublin

Abstract: Aortic coarctation is a congenital heart disease that has an incidence rate of 3-6 in every 10,000 live births. Currently, neonatal coarctation is treated surgically via a thoracotomy procedure, which involves excision of the narrowed section of the aorta followed by an end-to-end anastomosis to restore blood flow. For older children and adolescents, stenting is the procedure of choice. While stenting is associated with low instances of acute complications, there is a high risk of hypertension in the long term and possible aneurysm development. Due to the relatively small, yet complex, patient cohort and limited financial incentive for medical device companies, there is currently only one FDA approved stent for the treatment of aortic coarctation [6]. The aim of this work is to develop a framework to optimise the design and manufacture of 3D printed patient specific stents for aortic coarctation treatment."

3.21 Title: "Development of a Gene-Activated Biomimetic Scaffold Platform for Spinal Cord Injury Repair Applications (Poster)

Authors: Mullally, R, O'Connor, C, Dixon, E.J, Caldwell, M, Dervan, A, O'Brien, F.J

Affiliation: Royal College of Surgeons in Ireland

Abstract: Spinal cord injury (SCI) is a traumatic injury that induces permanent loss of function and paralysis. Repair is limited by the formation of a growth-inhibiting lesion cavity and the poor ability of damaged neurons to regrow their long axons. Biomaterial scaffold implants can bridge the lesion site, but few are optimised to actively support neuronal regrowth. Therefore, this project aims to develop a biomaterial scaffold carrying axon growth-inducing nucleic acid cargoes encapsulated in nanoparticles for non-viral gene delivery.

Here we show the optimisation of nanoparticle-encapsulated plasmid DNA for neuronal delivery and the successful development of a biomimetic scaffold platform, finely tuned to mimic the spinal cord's natural topography with optimised pore architecture, stiffness and composition. We demonstrate efficient nanoparticle-loading, yielding a gene-activated scaffold platform conducive for sustained gene delivery, neuronal uptake and growth. Gene-activated biomaterial scaffolds hold the potential to enhance and support axonal regrowth through the injured cord.

This work is funded by the SFI-AMBER Centre and IRFU-Charitable Trust.

3.22 Title: 2D Boron Nanosheets as an Osteogenic, Anti-Microbial and Mechanically Reinforcing Additive for Bone Tissue Engineering Scaffolds (Poster)

Authors: Jack Maughan, Harneet Kaur, Arlyng Gyveth Gonzalez-Vasquez, Lucy Prendeville, Tian Carey, Kevin Synnatschke, Ian Woods, Fergal J. O'Brien, Jonathan N. Coleman

Affiliation: Trinity College Dublin

Abstract: Bone repair is a multi-factorial problem, often requiring complex scaffolds to tackle inflammation and infection, all while enabling and improving osteogenesis, angiogenesis, neurogenesis and mechanical strength. In this work, we demonstrate the use of two-dimensional boron nanosheets, combined with collagen, to form a uniquely multi-functional bone scaffold tackling all of these problems simultaneously. Boron nanosheets were first synthesized and characterised, and these were then combined with collagen in film form and in porous scaffolds. Next, mechanical testing demonstrated the reinforcement of composite films by boron. Following this, the biocompatibility of the new boron-collagen material was established with bone cells, with a significant 43% increase in calcium deposition observed for the highest boron loading indicating a significant osteogenic effect. Further functional analysis using ELISA showed dose-dependent upregulation of angiogenic, anti-inflammatory, and neurogenic cytokines in the boron-collagen scaffolds. Finally, to further address concerns about infection, a significant anti-microbial effect was observed after testing with E. coli. These results clearly show that boron-collagen scaffolds can address multiple key regenerative targets simultaneously, and thus show significant potential as a platform for bone tissue engineering.

Materials for ICT

4.1 Title: Modulating Transition Metal Dichalcogenides properties through introducing impurities (Talk)

Authors: Cansu ilhan, Paul Hurley, Mick Morris.

Affiliation: Trinity College Dublin

Abstract: This study delves into the impact of varying impurity concentrations on the transport properties, and applicability of transition metal dichalcogenides (TMDCs), focusing on their semiconductor behavior. By employing thermally assisted conversion processes, this research leads the formation of both n-type and p-type TMDCs by converting transition metals into sulfide-based compounds at differing impurity levels. The TMDCs were subjected to 4-point resistivity and AC Hall-effect measurements to evaluate the semiconductor transport properties. Additionally, a comprehensive characterization of their structural, chemical, optical, and physical properties was conducted using techniques such as Raman spectroscopy, X-ray diffraction, UV-visible spectroscopy, and atomic force microscopy. The findings shed light on the profound influence of impurity concentrations on TMDCs, offering insights into their potential applications in thin-film technologies. This presentation will not only reveal the significance of impurity incorporation for optimizing the performance of TMDCs but also discuss the broader implications for their use in advanced electronic and optoelectronic devices.

4.2 Title: Separation of spin-orbit torque and thermal effects in Mn2RuGa (Talk)

Authors: Simon Lenne, Gwenaël Atcheson, Ross Smith, Plamen Stamenov, Karsten Rode

Affiliation: Trinity College Dublin

Abstract: There is growing interest in discovering new materials with strong spin-orbit torque (SOT), leading to the study of a wider range of magnetic materials. The harmonic Hall method is a commonly used technique for SOT measurement. However, this method is unable to distinguish between the Nernst effect and SOT. To address this, I developed an extension of the harmonic Hall method which allows for the accurate separation of Nernst and SOT effects. By simultaneously recording and analysing both the longitudinal and transverse signals, this method enables clear and precise separation of the SOT and the anomalous Nernst signals. Furthermore, the numerical implementation of this method enables the study of samples with a more complex anisotropy, such as Mn2RuGa. This approach allows for efficient measurement of SOT, even when signals are small or dominated by the Nernst effect. As a result, a greater diversity of potential materials can be analysed with accuracy."

4.3 Title: A reprogrammable metasurface for NIR beam steering and LiDAR applications (Talk)

Authors: Hodjat Hajian, and A. Louise Bradley

Affiliation: Trinity College Dublin

Abstract: Reprogrammable metasurfaces, spanning microwave to mid-infrared, offer active light modulation for communication, sensing, and imaging. Near-infrared electrically tunable metasurfaces are vital for LiDAR, demanding individual gating of nano-antennas and efficient heat management for stability and efficiency [1-2].

To this end, here we propose an electrically tunable Au-vanadium dioxide (VO2) metasurface on top of a one-dimensional Si-Al2O3 photonic crystal (PC), on a SiC substrate. Each individual Au-VO2 nano-antenna is switched from an Off to ON state via Joule heating, enabling the programming of the metasurface using 1-bit (binary) control with reflection efficiency at . While operating as a nearly perfect reflector at , the materials, thickness, and number of the layers in the PC are carefully chosen to ensure it acts as a thermal metamaterial. This enables efficient heat transfer from the Au nano-antennas to the SiC sink. The suggested design hold promise for LiDAR applications [2].

Acknowledgements

This research has emanated from projects supported by Science Foundation Ireland through 21/FFP-P/10187, AMBER 12/RC/2278 and IPIC 12/RC/2276.

References

[1] Park, B. Jeong, S. Kim, D. Lee, J. Kim, C. Shin, C. Lee, T. Otsuka, J. Kyoung, S. Kim, K. Yang, Y. Park, J. Lee, I. Hwang, J. Jang, S. Song, M. L. Brongersma, K. Ha, S. Hwang, H. Choo & B. Choi, “All-solid-state spatial light modulator with independent phase and amplitude control for three-dimensional LiDAR applications”, Nature Nano-technology 16, 69 (2021).

[2] M. Proffit, S. Pelivani, P. Landais, and A. L. Bradley, “Electrically Driven Reprogrammable Vanadium Dioxide Metasurface Using Binary Control for Broadband Beam Steering”, ACS Appl. Mater. Interfaces 14 41186–41195 (2022).

4.4 Title: What if the continuous large-area grown "monolayer" 2D material film is not just monolayer? (Talk)

Authors: Farzan Gity

Affiliation: University College Cork

Abstract: Localized electronic edge states in 2D nanostructures have critical impact in determining their material properties. Here, we report on experimental and theoretical investigations of $PtSe_2$ edge states, employing scanning tunneling microscopy and spectroscopy measurements, scanning transmission electron microscopy, as well as surface Green's function methodology in atomistic modeling of different edge atomic structures. Our results indicate that the edges can be semiconducting or semimetallic in nature depending on the edge configuration. Experimental results in conjunction with first-principles calculations demonstrate a mapped band profile of the atomically-sharp step edges of $PtSe_2$, revealing distinct electronic properties at such features inherent in polycrystalline films, which form lateral heterojunctions possessing large asymmetric band offsets in the conduction and valence bands. Such a monomaterial heterojunction is considered as the channel of a field-effect transistor, investigated by atomistic quantum transport simulations. This unveils the critical role of the edge states in creating a wider energy band for carrier transport in the ON-state and hence achieving a remarkably large I_{ON}/I_{OFF} ratio > 10^{10} and near-ideal subthreshold slope, fulfilling the requirements for low-power applications.

4.5 Title: Calculating the many-body density of states on a digital quantum computer (Poster)

Authors: Alessandro Summer, Cecilia Chiaracane, Mark T. Mitchison, and John Goold

Affiliation: Trinity College Dublin

Abstract: Quantum statistical mechanics allows us to extract thermodynamic information from a microscopic description of a many-body system. A key step is the calculation of the density of states, from which the partition function and all finite-temperature equilibrium thermodynamic quantities can be calculated. In this work, we devise and implement a quantum algorithm to perform an estimation of the density of states on a digital quantum computer which is inspired by the kernel polynomial method. Classically, the kernel polynomial method allows to sample spectral functions via a Chebyshev polynomial expansion. Our algorithm computes moments of the expansion on quantum hardware using a combination of random state preparation for stochastic trace evaluation and a controlled unitary operator. We use our algorithm to estimate the density of states of a non-integrable Hamiltonian on the Quantinuum H1-1 trapped ion chip for a controlled register of 18 qubits. This not only represents a state-of-the-art calculation of thermal properties of a many-body system on quantum hardware, but also exploits the controlled unitary evolution of a many-qubit register on an unprecedented scale.

4.6 Title: Growth and Characterisation of V2O5 and VOx Phase Mixtures for Memristive Device Applications (Poster)

Authors: Aisling Hussey, Brian Walls, Igor Shvets

Affiliation: Trinity College Dublin

Abstract: This study focuses on the growth and characterisation of vanadium oxides and their applications in memristive devices. Vanadium oxides have potential applications in devices for communication and computation, because their resistivity may be switched electrically, thermally and optically. Many vanadium oxides have metal to insulator transitions due to electron correlation effects. Vacuum annealing (10−6 mBar) of thin film V2O5 at 550C was shown to reduce the film to a mixed phase system containing V6O13. V2O5 was annealed for five and fifteen minutes. For the 15 minute annealed sample, the x-ray diffraction pattern contained peaks attributable to the V6O13 (001) family of planes, and the resistance was reduced. The metal to insulator transition of V6O13 was not observed indicating a mixed phase system.

4.7 Title: The critical role of ultra-low-energy vibrations in the relaxation dynamics of molecular qubits (Poster)

Authors: E Garlatti, A Albino, S Chicco, **VHA Nguyen**, F Santanni, L Paolasini, C Mazzoli, R Caciuffo, F Totti, P Santini, R Sessoli, A Lunghi, S Carretta

Affiliation: Trinity College Dublin

Abstract: Improving the performance of molecular qubits is a fundamental milestone towards unleashing the power of molecular magnetism in the second quantum revolution. Taming spin relaxation and decoherence due to vibrations is crucial to reach this milestone, but this is hindered by our lack of understanding on the nature of vibrations and their coupling to spins. Here we propose a synergistic approach to study a prototypical molecular qubit. It combines inelastic X-ray scattering to measure phonon dispersions along the main symmetry directions of the crystal and spin dynamics simulations based on DFT. We show that the canonical Debye picture of lattice dynamics breaks down and that intra-molecular vibrations with very-low energies of 1-2 meV are largely responsible for spin relaxation up to ambient temperature. We identify the origin of these modes, thus providing a rationale for improving spin coherence. The power and flexibility of our approach open new avenues for the investigation of magnetic molecules with the potential of removing roadblocks toward their use in quantum devices.

4.8 Title: Accurate and fast modelling of oxide bandgaps and defect levels from first principles DFT+U+J (Poster)

Authors: Daniel Lambert

Affiliation: Trinity College Dublin

Density functional theory (DFT) modelling of materials using the PBE or LDA functional is fast, but inaccurate at capturing bandgaps when compared to hybrid functionals. Linear response DFT+U+J is a technique that improves band gap accuracy by calculating both Hubbard U and Hunds J corrections from first principles.

In our research we benchmarked the performance of DFT+U+J against alternative methodologies such as hybrid functionals, observing their effect on bandgap accuracy and other properties for five oxide materials. We then modelled oxygen vacancies in TiO 2 , ZrO 2 , and HfO 2 using DFT+U+J, examining transition levels and defect formation energies.

It was found that DFT+U+J yields highly accurate band gaps, in some cases even outperforming hybrid functionals. This persists in O vacancy simulations, which show defect transition levels in line with previous research. This opens the route for first-principles, fast computation of band gaps and defect properties in large supercells."

4.9 Title: Sub-5 nm uniform zirconium oxide films on corrugated copper substrates: Polymer Brush Assisted Deposition for Advanced Semiconductor Technology (Poster)

Authors: Sajan Singh, Pravind Yadav, Michael Morris

Affiliation: Trinity College Dublin

Abstract: Fabricating ultrathin dielectric films, especially those with high dielectric constants, is crucial for various advanced applications like protective coatings, sensors, and next-gen logic devices. The current state-of-the-art in microelectronics for fabricating these thin films is a combination of combining atomic layer deposition (ALD) and photolithography. The continual reduction in electronic device size has led to challenges in top-down photolithography approaches. This, along with increasing circuit complexity, has driven the demand for controlled deposition of nanoscale materials via bottom-up methods.

Here, we propose a novel method using polymer brush templates for depositing continuous, uniform zirconium oxide (ZrO2) films on copper (Cu) substrates. By employing thiol-terminated polymethyl methacrylate brush (PMMA-SH) as a template, we enable selective infiltration of zirconium oxynitrate (ZrN2O7), ensuring pin-hole free films. Achieving a uniform polymer monolayer on the Cu substrate is critical for consistent film thickness. Chemical interactions between the polymer functional group and the metal precursor facilitate infiltration, followed by a reductive H2 plasma treatment to form the ZrO2 film. Analysis through XPS, GA-FTIR, cross-sectional transmission electron microscopy, and energy-dispersive X-ray mapping confirms ZrO2 formation at the Cu substrate.

This methodology offers a scalable approach for preparing ZrO2 films, which could extend to other high-κ dielectric materials, promising advancements in microelectronic applications.

4.10 Title: Slow and Fast Light Transition in Coupled Waveguide-ENZ Modes (Poster)

Authors: Edward H Krock, John F. Donegan

Affiliation: Trinity College Dublin

Abstract: Research in the last decade has demonstrated the ability to dramatic increase, reduce or change the direction of the group velocity of light, referred to as fast or slow light [1]. This tunability originates from the dispersion properties of a material medium or structural resonances such as photonics crystals or plasmonics [2]. Epsilon Near Zero (ENZ) modes are plasmonic resonances at the ENZ point, where the real part of the electric permittivity vanishes [3]. This vanishing permittivity result in unusual physics such infinite phase velocities [4] and slow light [5].

In this work, we investigated the group velocity of the first two (n=1,2) coupled waveguide-ENZ modes at the ENZ wavelength of Indium Tin Oxide (ITO). Using Lumerical FDE, we modelled a multilayer stack of SiO2 substrate- ITO- 1500 nm PMMA at 1226 nm. We investigated the properties of the n=1 and n=2 modes, demonstrating variations in group velocity with varying thickness of ITO from 20-30 nm.

By extracting the shape of the modes, we show the existence of coupled waveguide-ENZ modes. Increasing the thickness of the ITO layer, the group velocity of the n=1 mode is approximately constant at 0.5c. For thicknesses larger than 22.5 nms, the n=2 mode displays fast light in the same direction as the incident beam. At 22.5 nms, we observed a transition to zero group velocity and below 22.5 nms, the group velocity becomes negative. This negative group velocity would result in the peak of a transmitted pulse leaving the medium before the peak enters the medium, if the large losses are compensated for. However, it is important to note that only the peaks would appear to travel in the opposite direction, as the power flow is still in the positive direction. [6] We hypothesis this result comes from the interference between ENZ and waveguide modes. Similar interference effects have been demonstrated in plasmonic structures relying on Fano Resonances

between plasmonic modes [7,8,9]. These results demonstrate the ability to significantly vary the group velocity in simple multilayer structures by tuning the ITO thickness.

REFERENCES

[1] Boyd, R W.," Slow and Fast Light: Fundamentals and Applications" Journal of Modern Optics.56:18-19, 1908-1915 (2009).
[2] Boyd, R W.," "Material slow light and structural slow light: similarities and differences for nonlinear optics [Invited]" J.Opt.Soc Am. B Vol. 28,No.12 (2011).
[3] Campione, S., Brener, I. and Marquier, F. "Theory of epsilon-near-zero modes in ultrathin films".Phys. Rev. B 91,121408(R) (2015)
[4] Liberal, I., Engheta, N., "Near-zero refractive index photonics" Nature photonics, 11,149-158 (2017).
[5] Bello, F., Page, A.F., Pusch, A. et al. "Combining ε-Near-Zero Behavior and Stopped Light Energy Bands for Ultra-Low Reflection and Reduced Dispersion of Slow Light". Sci Rep 7, 8702 (2017).
[6] George M. Gehring, et al., "Observation of Backward Pulse Propagation Through a Medium with a Negative Group Velocity". Science 321, 895-897 (2006).
[7] Yundong Zhang, Xuenan Zhang, Ying Wang, Ruidong Zhu, Yulong Gai, Xiaoqi Liu, and Ping Yuan, ""Reversible Fano resonance by transition from fast light to slow light in a coupled-resonator-induced transparency structure,"" Opt. Express 21, 8570-8586 (2013)

[8] El Haffar, R., Farkhsi, A. & Mahboub, O. Optical properties of MIM plasmonic waveguide with an elliptical cavity resonator. Appl. Phys. A 126, 486 (2020).
[9] Wu, C., Khanikaev, A B. & Shvets, G. “Broadband Slow Light Metamaterial Based on a DoubleContinuum Fano Resonance”. Phys. Rev. Lett. 106,107403 (2011"

4.11 Title: Exploring the Potential of Spatially Variant Plasmonic Gratings (SVPGs) in Advancing Light Manipulation Technologies (Poster)

Authors: Mugahid Ali*, Edward Krock, and John Donegan

Affiliation: Trinity College Dublin

Abstract: Spatially variant plasmonic gratings (SVPGs) represent a cutting-edge platform in photonics and plasmonic applications, offering unique tunable and polarisation-dependent optical properties. They can enhance the electromagnetic field across large areas exceeding a micrometre scale (10^{-6}m), a significant leap beyond conventional plasmonic devices limited to nanometer-scale regions (10^{-9}m) (Figure 1). This study underscores the multifaceted adaptability of SVPGs, particularly their straightforward fabrication processes, seamless integration with 2D materials featuring electrically tunable properties such as graphene and MoS2, and polarisation-dependant enhancement of the spontaneous emission via the Purcell effect. It also elucidates the theoretical underpinnings and validations of SVPGs, showcasing their potential to redefine photonics platforms by fostering efficient, polarisation-dependant and spatially controlled light-matter interactions. We envisage this to unveil new prospects for designing advanced photonic and plasmonic devices with enhanced functionalities, heralding a transformative paradigm in photonics research and application, particularly for single-emitter-based cavity quantum electrodynamics.

4.12 Title: Spintronic properties of RuO2/TiO2 MTJs MTJs (Poster)

Authors: Willy LABORDE, Dr. Maria Stamenova and Professor Stefano Sanvito

Affiliation: Trinity College Dublin

Abstract: Altermagnetism is a new predicted phase of magnetism using magnetic group theory applied to decoupled crystallographic and spin space [1]. It is now being seen as a third phase of magnetism alongside with ferromagnetism and Antiferromagnetism. In the context of spintronics devices, altermagnetism has all the physical advantages of antiferromagnetism, e.g. zero net magnetic moment or robust to external magnetic fields perturbation and magnetic probes. The most important feature is a spin-splitting of the electronic band structure in such class of magnets. These can allow for the use of globally non-spin polarised current for conventional spintronic applications. We can exploit such novel material properties to design new spintronic prototypes, study their spin-transport properties and open the way to a new pioneering physics. We designed several altermagnetic multilayer devices based on the symmetry principles for this new phase of magnetism. The spin-splitting of the band structure can be exploited to produce spintronic

effects of interest as the tunnelling magneto-resistance (TMR) and the spin-transfer torque (STT). We're currently extending our investigation to finite bias and finite temperature effects. These promising non-conventional MTJs based on AFM materials exhibiting a strong non-spin-orbit-related spin-splitting need to be studied microscopically from first-principles theory. One promising device candidate RuO_2 / TiO_2 / RuO_2 has been recently proposed giving a TMR ratio in excess of 500% at zero bias [2]. We recently confirmed this result qualitatively. However, we extended the results by exploring the finite bias regime and the second key spintronic effect, the spin-transfer torque (STT). Our preliminary results showed that producing accurate results is very sensitive to numerical detail in the material modeling, also because of the instable nature of RuO_2. We also aim to present novel results on other altermagnetic prototypes we designed.

Sustainable Functional Materials

5.1 Title: Yeast surface codisplay of PETase, MHETase and hydrophobin as a whole-cell biocatalyst for the degradation of PET (Talk)

Authors: Vanja Juric, Justin Holmes

Affiliation: University College Cork

Abstract: Traditional plastics such as PET are usually not biodegradable, and plastic waste accumulates and contaminates natural environments. They fragment into particles smaller than 5 mm, known as microplastics, which damage marine ecosystems and pose serious risks to human health. Significant greenhouse gas emissions are generated across the life cycle of plastics, beginning with production and concluding with incineration. Bio-based synthesis and recycling of plastics can reduce fossil fuel use and CO2 emissions. This project focuses on the production of enzymes involved in plastics degradation. The yeast MoClo (modular cloning) toolkit was modified to enable the efficient incorporation of a panel of five surface display anchor proteins into Saccharomyces cerevisiae expression cassettes, thereby enabling the enzymes to be displayed on the outside surface of yeast cells, with the goal of using the yeast cells as whole cell catalysts. The display anchors were initially validated using two proteins of interest. Subsequently, the toolkit enabled the successful expression of PETase and MHETase, enzymes which degrade polyethylene terephthalate and mono-2-hydroxyethyl terephthalate, respectively, as well as the expression of hydrophobin, a protein that facilitates attachment of yeast cells to hydrophobic surfaces such as PET. Going forward, the yeast cells with displayed proteins will be tested for activity on PET under different conditions and compared with other methods for degrading PET with enzymes.

5.2 Title: The presence of disorder is ubiquitous in the manufacturing of graphene and graphene nanodevices. (Talk)

Authors: Shardul Mukim, Fabio Duarte and Prof. Mauro S. Ferreira

Affiliation: Trinity College Dublin

Abstract: Computationally it is a straightforward task to get electronic signatures of such devices if complete information about the underlying Hamiltonian is available. However, to do so in reverse is a difficult task in the presence of disorders. In this article, we apply a recently developed inversion technique to identify important structural information of the zigzag-edged graphene nanoribbon. The inversion tool decodes the transmission spectrum to yield the concentration and the asymmetry in the occupation of vacancies of the zigzag-edged graphene nanoribbon. We apply spin-polarised transmissions to the test and show that the inversion procedure can indeed detect the edge roughness and magnetism of the graphene nanoribbon.

We also go on to show that spin-polarised transmission of a particular orientation is sufficient to derive all the structural information about the device."

5.3 Title: Functionalised electrospun nanofibrous membranes for selective separation applications (Talk)

Authors: Saranya Rameshkumar, Ramesh Babu

Affiliation: Trinity College Dublin

Abstract: Surface-functionalised polymeric nanofiber membranes were fabricated using electrospinning method to achieve high-throughput selective separation of valuable organic solutes from fermentation products/bio-refineries. Based on optimised polymer solution properties and electrospinning operating conditions, mechanically stable electrospun membranes of polyether sulfone (PES) and crosslinked PES are fabricated with uniform fiber diameter of nearly 1 micron and 300 nm respectively. Novel surface modification approaches based on co-polymer functionalisation, in-situ cross-linking, surface polymerisation using electrospraying have been explored to create surface-selective functional layer on top of PES electrospun membranes. Initial studies on polymer blending using hydroxypropyl b-cyclodextrin (HPBCD) as a functional moiety has offered to produce smooth, uniform and reproducible nanofibers of ~300 nm fiber diameter. Under optimised conditions, PES/HPBCD crosslinked electrospun membrane of nearly 80-100-micron thickness were produced with improved wettability and hydrophilic characteristics. Surface functionalisation was attempted using 2D nanomaterials like conductive graphene ink and molybdenum sulfide to form thin selective layer on the nanofibrous membrane surface. Functionalised electrospun membranes with superior pore and surface characteristics have been developed to achieve improved rejection efficiency with lesser trade-off on the permeation flux. Performance evaluation of developed electrospun membranes is being carried out to benchmark its permeation and rejection efficiency with commercial ultrafiltration membranes in selectively separating out sugars from dairy process streams.

5.4 Title: Diblock Polypeptide Hydrogels as Bioinks for 3D Printing in Tissue Engineering (Talk)

Authors: Muireann Cosgrave, Robert Murphy, Kulwinder Kaur, Chris Simpson, Ciara Murphy and Andreas Heise

Affiliation: Royal College of Surgeons in Ireland

Abstract: The use of 3D printing in tissue engineering (bio-printing) has rapidly increased throughout recent years, namely due to its ability to construct more complex, cell-viable 3D structures.1 Hydrogels are a prominent choice for bio-ink formulations as they can be engineered to simulate the native extracellular matrix (ECM).2 Furthermore, their mechanical properties can

be altered to optimize printability and cytocompatibility properties. For particular applications, the choice of hydrogel used in bio-printing processes encompasses several important considerations, particularly that its strength is stable and suitable for the printing process, whilst also being comparable in strength to that of the native tissue it is replacing.

Here we present a range of amphiphilic star-shaped diblock co-polypeptides consisting of methacrylamide functionalized poly(L-glutamate)-b-(L-leucine) with different star architectures. The hydrophobic side chains of the L-leucine blocks drive the self-assembly of the polypeptides in water, spontaneously forming stable hydrogels. The mechanical properties of these materials are readily tuned by varying the star architecture and the monomer feed used. They also possess shear-thinning and self recovery properties, indicating their suitability for extrusion based 3D printing. Complex 3D printed structures can be readily generated and then photo-crosslinked using visible light (405 nm) in the presence of comonomers. Printed hydrogels show good biocompatibility and represent viable bio-ink material platforms for tissue engineering.

References

(1) Li, J.; Wu, C.; Chu, P. K.; Gelinsky, M. 3D Printing of Hydrogels: Rational Design Strategies and Emerging Biomedical Applications. Mater. Sci. Eng. R Rep. 2020, 140, 100543. https://doi.org/10.1016/j.mser.2020.100543.
(2) Ramiah, P.; du Toit, L. C.; Choonara, Y. E.; Kondiah, P. P. D.; Pillay, V. Hydrogel-Based Bioinks for 3D Bioprinting in Tissue Regeneration. Front. Mater. 2020, 7, 76. https://doi.org/10.3389/fmats.2020.00076."

5.5 Title: The Synthesis of Mechanically Interlocking Molecules using the btp [2,6- bis(1,2,3-triazole-4-yl)pyridine] motif (Poster)

Authors: Niamh A O'Shea, Patrick J. Manning, Bláithín Rawson, Owen Oseghale, and Thorfinnur Gunnlaugsson

Affiliation: Trinity College Dublin

Abstract: The world of mechanically interlocking molecules (MIMs) has gained providence since the 2016 Nobel Prize Awards, for which Stoddart and Sauvage received the prize for their pioneering work on molecular machines. Rotaxanes are becoming a more and more prominent MIM in the world of mechanostereochemistry due to their versatility and their never-ending potential. Rotaxanes comprise a ring and a dumbbell component; these components are noncovalently bonded, but to break these components apart, a covalent bond must be broken. Previously, the Gunnlaugsson Group have successfully synthesised btp [2,6-bis(1,2,3-triazole-4-yl)pyridine] macrocycles and catenanes (Byrne et al., 2014) (see figure 1 for synthesis plan) but have yet to look at rotaxanes. The formation Herein, we present work based upon the btp binding motif, including psueodorotaxanes and various macrocycles synthesised through click chemistry. Whilst also presenting synthesis work on creating selective macrocycle conditions for one of the group's btp macrocycles. We will also present work on the use of lanthanide metals with

interlocking molecules (Molloy et al., 2012). This project aims to produce and create novel interlocking molecule materials for use within the electronic, imaging, and magnetic industries whilst also aiming to utilize these structures in the formation of 'all organic-based redox-active materials for use in batteries.

1 J. P. Byrne, J. A. Kitchen, O. Kotova, V. Leigh, A. P. Bell, J. J. Boland, M. Albrecht and T. Gunnlaugsson, Dalton Trans., 2014, 43, 196–209.
2. J. K. Molloy, O. Kotova, R. D. Peacock and T. Gunnlaugsson, Org. Biomol. Chem., 2012, 10, 314–322.

5.6 Title: Naphthalimides Exhibiting Aggregation Induced Emission For Bioimaging: Applications in Biomaterials (Poster)

Authors: L. Constance Sigurvinsson, Adam F. Henwood, Niamh Curtin, Tómas Gudmundsson, Deirdre McAdams, Donal F. O'Shea and Thorfinnur Gunnlaugsson

Affiliation: Trinity College Dublin

Abstract: A 1,8-naphthalimide (Nap) is functionalised with triphenylamino (TPA) moieties which, by virtue of having multiple freely rotating aromatic rings, are capable of exhibiting aggregation induced emission (AIE) in aqueous environments. The synthesis of this Nap is undertaken via a double Suzuki-Miyaura coupling procedure and the compound is characterised using 1H and 13C NMR, IR, mass spectrometry, elemental analysis, and by single crystal X-ray diffraction. Photophysical studies reveal that the emission of this TPA Nap is bluer and more emissive in apolar solvents, emitting from a planarized charge transfer (CT) state, while the emission redshifts and becomes quenched in polar media as it adopts a twisted intramolecular charge transfer state (TICT). In THF the molecule is emissive but upon addition of water, the fluorescence is immediately quenched. However, at a critical water content (>70% water in THF), the TPA Nap once again becomes luminescent due to AIE becoming the dominant process.

5.7 Title: Digital Light Processing 3D Printing of Caprolactone Copolymers with Tailored Properties through Crystallinity (Poster)

Authors: Gianluca Bartolini Torres, Bo Li and Andreas Heise

Affiliation: Royal College of Surgeons in Ireland

Abstract: Digital light processing (DLP) 3D printing has shown great advantages in the fabrication of 3D objects towards various applications. As a biocompatible material, post-functionalised PCL has been demonstrated as a promising candidate for DLP printing, while the mechanical properties mainly relied on molecular weight and crosslinking density. Herein, we introduced a copolymerisation of caprolactones offering built-in functionality for photochemistry. By altering the monomer feeding, a crystalline block copolymer and an amorphous random copolymer were obtained. DLP printed scaffolds from these copolymers have inherited their thermal properties,

leading to dramatic different mechanical properties. Moreover, the crystalline scaffold displayed a shape memory property as the first example of PCL copolymer in DLP printing. This work has offered the simplicity of achieving photo reactivity, tailored mechanical properties and shape memory for DLP printing from two straightforward copolymerisations.

5.8 Title: "PtSe2/graphene hybrids with enhanced HER performance (Poster)

Authors: Ilias M. Oikonomou, Apostolos Koutsioukis, Thomas Brumme, Axel Zuber, Clive Downing, Zdenek Sofer, Michelle Browne, Thomas Heine and Valeria Nicolosi

Affiliation: Trinity College Dublin

Abstract: Liquid phase exfoliation (LPE) is the most effective way of producing two-dimensional materials inks, through a sustainable and cost-effective procedure. PtSe2, which belongs to noble-metal chalcogenides, has a broad range of applications in photonics, sensing, and catalysis. However, the cost of platinum is a critical aspect of large-scale production in energy applications. In this work, we present the fabrication of PtSe2/graphene hybrids using LPE. Density functional theory was used to quantify the interaction between the two materials by calculating the binding energy of graphene on PtSe2. The structural features of the samples were identified with conventional Transmission Electron Microscopy (TEM), selected area electron diffraction, and scanning-TEM accompanied by elemental mapping. UV-visible and Raman spectroscopy were both utilized to unravel optical and vibrational properties. The hybrid system has enhanced conductivity and reduced overpotential for Hydrogen evolution reaction (HER) in comparison with the separate materials.

5.9 Title: Creation of coatings that form barriers to enhance the barrier qualities of eco-friendly beverage packaging options (Poster)

Authors: Hossein Rajabinejad, Prof Michael Morris

Affiliation: Trinity College Dublin

Abstract: The core scientific challenge of this project lies in the development of pioneering barrier-forming coatings aimed at amplifying the sustainability and functionality of packaging materials specifically designed for both carbonated and non-carbonated beverages. This endeavor seeks to cater to the escalating demand for eco-friendly packaging solutions that not only preserve the quality of the product but also minimize environmental impact and promote recyclability. By incorporating sustainable materials into the creation of these innovative coatings, the project endeavors to set new benchmarks in the packaging industry, ensuring that environmental stewardship and superior product integrity go hand in hand.

5.10 Title: PACBED Contrast Enhancement via STEM Beam Modulation (Poster)

Authors: Matthew Mosse, Jonathan J P Peters, Shelly Conroy, Lewys Jones

Affiliation: Trinity College Dublin

Abstract: Scanning transmission electron microscope (STEM) detectors output analogue signals, but by digitising this signal new dose-saving strategies are possible.

Combining the ability to count electrons in real time with an electrostatic shutter, a new imaging mode is produced. Instead of counting the number of electrons in a given time, the time for a set number of electrons is measured and the beam is blanked, reducing the overall dose.

Additionally, by collecting equal numbers of electrons from more and less scattering areas, dose is placed on areas which will produce less heating and damage. Secondly, the signal is weighted more towards lighter elements that would normally have lower signal-to-noise ratio.

Here, the effect on PACBED imaging is investigated by simulation. It is proposed that fine-details would be emphasised in the diffraction patterns, producing higher contrast and better signal-to-noise ratio in PACBED with this new mode.

5.11 Title: Direct Laser Writing of Electro-Actuating Microstructures (Poster)

Authors: Jason M. Delente, Srikanth Kolagatla, Donagh Mc Ginley, Colm Delaney, Larisa Florea

Affiliation: Trinity College Dublin

Abstract: Stimuli-responsive hydrogels are highly attractive materials as they can be studied in aqueous environments, are easily functionalised to respond to specific stimuli and enable the diffusion of the solvent/analytes within their structures. Electro-active hydrogels are gels that convert the energy of an applied electric field to a mechanical motion through several mechanisms which can operate simultaneously. One of the major drawbacks of macroscale actuators is that they usually demonstrate slow actuation which limits their use. By using two-photon polymerisation (TPP), a direct laser writing technique which enables the fabrication of complex 3D polymer microstructures, successful fabrication of electro-actuating microstructures which could actuate faster than their macroscale counterparts was achieved.

Herein is presented the fabrication of electro-actuating microstructures by TPP, with an in-depth study of their properties along with the influence of several factors on the electro-actuation (variation of pH, concentration of electrolyte, position relative to the electrode and potential applied).

5.12 Title: An Engaged Research Approach in Materials Science and Technology Projects: Perspectives from Key Stakeholders (Poster)

Authors: Sadhbh Crean, Dr. Amy Fahy, Dr. Joseph Roche and Professor Mick Morris.

Affiliation: Trinity College Dublin

Abstract: Aligning with international calls for participatory science to enhance the voice of the public across science, technology, and knowledge-production (Campus Engage Ireland, 2022; Robinson et al., 2021; SFI, 2021), this research presents a case study of how multi-stakeholder, quadruple helix (Carayannis & Campbell, 2009), Engaged Research is perceived and operationalised to maximise societal and environmental impact within research projects at the Science Foundation Ireland Research Centre for Advanced Materials and Bioengineering Research (AMBER) and beyond. Engaged Research refers to a broad range of research approaches and methodologies that involve working with multiple stakeholders (Holliman, 2017). A qualitative research design was implemented, collecting data from participants using semi-structured interviews and following an iterative research process (Hoffman et al., 2019). This poster outlines the key challenges and drivers of forming inclusive, cross-disciplinary relationships, co-creating, and acting on collaborative goals to address societal challenges, and multi-stakeholder participation from research conception to evaluation and dissemination.

5.13 Title: Fabrication of sub-20 nm MoS2 horizontal nanowire arrays by block copolymer assisted inclusion method (Poster)

Authors: Tandra Ghoshal, Michael A. Morris

Affiliation: Trinity College Dublin

Abstract: We demonstrate the fabrication of sub-20 nm MoS2 horizontal nanowire arrays on silicon substrates using self-assembled block copolymer assisted insitu inclusion approach. Microphase separated long range ordered polystyrene-b-polyethylene oxide (PS-b-PEO) block copolymer line nanopatterns were achieved through thermo-solvent annealing. The BCP structures were etched/modified by anhydrous ethanol to facilitate insertion of molybdenum precursor within the film. Horizontal ordered molybdenum oxide nanowire arrays were fabricated by UV/Ozone treatment. The oxides were converted to sulphides by thermal evaporation at different temperatures by Ar/ H2 environment. XPS revealed the composition and phases of molybdenum oxide and sulphide nanowires. Elemental mapping was performed to investigate the interfaces. The formation and stability of the sulphide nanowires were studied at different temperatures. The photoluminescence and Raman properties were studied at different formation temperatures to investigate defects and estimate the numbers of layers.

5.14 Title: Anti-Icing Properties of Polar Bear Fur (Poster)

Authors: Julian Carolan, Martin Jakubec, Neubi F. Xavier, Jr, Adam Pestana Motala, Ersilia Bifulco, Jon Aars, Magnus Andersen, Anne Lisbeth Schmidt, Marc Brunet Cabre, Vikaramjeet Singh, Paula E. Colavita, Espen Werdal Selfors, Marco Sacchi, Shane O'Reilly, Øyvind Halskau, Manish Tiwari, Richard G.Hobbs and Bodil Holst

Affiliation: Trinity College Dublin

Abstract: The project seeks to produce passive anti-icing surfaces taking inspiration from Arctic animals such as Arctic foxes, Arctic hares, and polar bears. Such passive anti-icing surfaces would be critical for advances in aerospace materials and air conditioning where they would allow significant energy savings over current de-icing treatments. Inspiration has been taken from these animals as they display water repellency and anti-icing properties despite animals such as polar bears swimming large distances and sliding on snow. By understanding these mechanisms by which polar bears and penguins negate ice build up we hope to design materials which will have the same properties or better for use in our daily lives.

5.15 Title: Production of Biobased Polymers (PET, PHFA and PAFA) from Lignin (Poster)

Authors: Hamid Hafizi, Bilal Ul Amin, Maurice N. Collins

Affiliation: University of Limerick

Abstract: Lignocellulosic biomass has three main components: cellulose, hemicellulose, and lignin. Cellulose comprises 30–50% of biomass, depending on the plant species, and is a polymer of glucose. A smaller portion, 20–35%, is hemicellulose, which is a heteropolymer containing primarily xylose. Lignin accounts for the remaining 15–30% of biomass and is a cross-linked, aromatic-based heteropolymer. Lignin is an amorphous polymer containing phenolic monomers. As the second most abundant natural polymer, lignin is the only scalable renewable feedstock but is highly underutilized. In this project we are working on the production of lignin-based polyethylene terephthalate (PET) and also poly(dihydroferulicacid)(PHFA) and poly(acetylferulic acid)(PAFA), which are effective PET mimics, as potential sustainable alternatives to petroleum-based polymers. Lignin was extracted from biomass waste and then depolymerized into its constituent monomers. Subsequently, purification of these monomers and their conversion via a cascade catalytic process enables synthesis of building blocks for polymerization into PET, PHFA and PAFA.

5.16 Title: Upstream Recovery of Phosphates From Dairy Processing Wastewater (Poster)

Authors: Dr. Mukesh Pednekar and Prof. Ramesh Babu Padamati

Affiliation: Trinity College Dublin

Abstract: Phosphorus is an essential nutrient in plant growth and an important component in the food supply chain. However, excessive phosphorus discharge into water bodies through wastewater has led to eutrophication and poses significant environmental problems. Recovery of phosphate from wastewater prevents phosphorus from entering water bodies and provides phosphate-based products. Our research focused on recovering phosphate from dairy processing wastewater, conventionally treated using a combination of chemical and biological processes for the regulatory compliance. Dairy wastewater treatment involves energy-intensive processes and excessive use of chemicals that generate large volumes of low-value sludges. We are working to recover phosphate from dairy wastewater in a commercially suitable form while overcoming

industrial challenges. Overall, our research provides an upstream phosphate recovery approach for mitigating environmental impacts with resource conservation and improving industrial sustainability.

5.17 Title: Static friction at the microscale investigated at the limit of Hertzian pressure by oscillatory shear experiments (Poster)

Authors: Ahmed Uluca, Rui Dong, Stefano Sanvito, Graham L.W. Cross

Affiliation: Trinity College Dublin

Abstract: The force to initiate relative motion between contacting bodies -the static friction force- has been investigated with a novel 2-dimensional nano-indenter setup (©KLA Gemini) for a single micrometer scale asperity. Both normal load and stiffness (contact area) are monitored while simultaneously applying an oscillatory sheer force of controlled amplitude. A decrease from a full stick zone elastic response to fully sliding expected from Mindlin's sheared contact model have been demonstrated during the increase of the shear force. Accordingly, a static friction force is calculated by asymptote to zero stiffness. Static friction coefficients have been shown to be decreased by increasing load which we explain by correlating the friction force with interfacial shear strength (ISS) and contact area. Therefore, up to the onset of plasticity, the contact area and load obeys Hertzian relations that should yield a decreasing static friction coefficient by an inverse root cube proportionality to load.

5.18 Title: Fully sustainable PET derived from terephthalic acid produced from lignocellulosic waste (Poster)

Authors: Hamid Hafizi, Bilal ul Amin, Maurice Collins

Affiliation: University of Limerick

Abstract: Lignocellulosic biomass has three main components: cellulose, hemicellulose, and lignin. Cellulose comprises 30− 50% of biomass, depending on the plant species, and is a polymer of glucose. A smaller portion, 20−35%, is hemicellulose, which is a heteropolymer containing primarily xylose. Lignin accounts for the remaining 15−30% of biomass and is a cross-linked, aromatic-based heteropolymer. Lignin is an amorphous polymer containing phenolic monomers. As the second most abundant natural polymer, lignin is the only scalable renewable feedstock but is highly underutilized. In this project we are working on the production of lignin-based polyethylene terephthalate (PET) and also poly(dihydroferulicacid)(PHFA) and poly(acetylferulic acid)(PAFA), which are effective PET mimics, as potential sustainable alternatives to petroleum-based polymers. Lignin was extracted from biomass waste and then depolymerized into its constituent monomers. Subsequently, purification of these monomers and their conversion via a cascade catalytic process enables synthesis of building blocks for polymerization into PET, PHFA and PAFA.

5.19 Title: Insights into cyanoacrylates polymerization (Poster)

Authors: Josué M. Galindo, Agnieszka Ciechacka, Cormac Duffy, Deborah Coleman, Paul O'Donohue, Niamh Cronly, Barry Burns, Andreas Heise

Affiliation: Royal College of Surgeons in Ireland

Abstract: Cyanoacrylates (CAs) are widely recognized as fast-setting adhesives, commonly available in liquid form with stabilizers. Instant adhesion occurs through rapid anionic polymerization triggered by surface moisture exposure. However, there is a growing interest in exploring the crosslinking process via radical polymerization. Here is a summary of the primary CA and resulting polymers, beginning with an in-depth examination of monomer and polymer traits as documented in the literature. Subsequently, this discussion delves into the investigations surrounding radical homo- and copolymerization.

5.20 Title: Next generation 3D printed photonic structures (Poster)

Authors: Jamie Somers, Jing Qian, Colm Delaney, Jang Ah Kim, Alex J. Thompson and A. Louise Bradley.
Affiliation: Trinity College Dublin

Abstract: Two-photon polymerisation (2PP) was first theorised by Göppert-Mayer all the way back in 1931, and has been of interest to researchers in material science since the invention of the laser all the way back in 1960. Over the past number of years chemists have been working to engineer materials which can be used for 3D printing via 2PP. Today this revolutionary technique of printing is combined with responsive hydrogels. Despite their low refractive index these photoresists can print complex photonic structures which display bright saturated colour by replicating structures found in nature. Butterfly wings, beetles and chameleons all rely on "structural colour" to produce their vibrant and eye-catching chromaticity. The goal of this project is to use a novel technique of printing responsive structures on the distal end of an optical fibre to produce sensors which use the phenomenon of structural colour in response to stimuli.

5.21 Title: Morphological characterisation of printed networks of nano-materials using 3D FIB-SEM nanotomography (Poster)

Authors: Doolan, Luke, Gabbett, Cian, Synnatschke, Kevin, Gambini, Laura, Coleman, Emmet, G. Kelly, Adam, Liu, Shixin, Caffrey, Eoin, Munuera, Jose, Murphy, Catriona, Sanvito, Stefano, Jones, Lewys, Coleman, Jonathan N

Affiliation: Trinity College Dublin

Abstract: Networks of nanomaterials show great promise for printed electronic devices. While it is known that network morphology plays a dominant role in determining the physical properties of printed nanomaterial devices, quantitative measurements of morphology have proven difficult. Focused-ion-beam scanning-electron-microscope nanotomography (FIB-SEM nt) can be used to create 3D images of representative volumes of printed networks with nanometre resolution. FIB-SEM nt was used to image printed networks of graphene with different nanosheet length. Using machine learning, 3D images were segmented and different morphological properties of the networks, including porosity, nanosheet alignment, along with pore and nanosheet tortuosity were calculated. These properties were used to model the effect of nanosheet length on the electrical properties of the network. FIB-SEM nt was also applied to printed networks composed of silver nanoplatelets, silver nanowires and tungsten disulphide. Finally, the technique was applied to printed devices, allowing the calculation of interfacial roughness within printed heterostacks.

5.22 Title: Micro-Actuators with pH-Responsive Hydrogel via Two-Photon Polymerisation (Poster)

Authors: Yekaterina Tskhe, Srikanth Kolagatla, Colm Delaney, Larisa Florea

Affiliation: Trinity College Dublin

Abstract: Additive manufacturing in micro-robotics offers promising potential for microscale smart device development, showcasing precise control for object manipulation. This work focuses on fabricating multi-material 3D micro-actuators via direct laser writing using two-photon polymerization (2PP). This technique enables the construction of intricate 3D microstructures by moving a focused femtosecond laser beam across polymer hydrogels, allowing for tailored chemical and mechanical properties. Actuation is achieved using pH-responsive polymer hydrogels, inspired by artificial muscles. The response takes only a few seconds due to their miniature size. Incorporating two types of pH-responsive hydrogels enables the creation of pH sorter microsystem. Performance optimization is explored through design, hydrogel compositions, and fabrication parameters analyzed using optical microscopy, atomic force microscopy (AFM), and scanning electron microscopy (SEM). The presented approach demonstrates the controlled fabrication of novel programmable 4D micro-tools integrated with stimuli-responsive materials, creating opportunities for advanced sensing and microfluidics applications.

5.23 Title: The effect of nanosheet dimensions on nanosheet network charge transport (Poster)

Authors: Anthony Dawson, Jonathan Coleman

Affiliation: Trinity College Dublin

Abstract: Printed devices are formed of networks of nanosheets contacting one another at junctions. This work outlines the role of nanosheet dimensions in dictating the electronic properties of these nanosheet networks. If widespread integration of printed electronics is to be realized, it is vital that we first fully understand charge transport through networks and optimize this. Here, we have developed a novel method to control nanosheet dimensions while keeping nanosheet thickness mostly unchanged, enabling the tuning of nanosheet length to thickness ratio between 100 and 450. Utilizing tip induced scission, this process is scalable, and relatively straightforward.

Size selected devices were produced from this material, and their DC conductivity compared to expectations from a recently published network conductivity equation. It was found that that maximizing nanosheet area will maximize network conductivity. This demonstrates substantial progress in understanding network properties dictated by nanosheet dimensions.

5.24 Title: Surface Modification of PET Films for Food Packaging Applications (Poster)

Authors: Sukhananazerin Abdulla, Sibu C Padmanabhan, Malco-Cruz Romero, Joseph P Kerry, Michael A Morris

Affiliation: Trinity College Dublin

Abstract: In the packaging industry, Polyethylene terephthalate (PET) is one of the most used polymers due to its lightweight, flexible, biocompatibility, mechanical strength, high transparency, and resistance against chemicals and/or abrasion. However, poor gas barrier properties and antimicrobial activity are still unsolved challenges, which limit its application in the food packaging industry. Thus, surface modification of PET films using active functionalities is often required for a wide range of applications. To this aim, our project is focused on the development of surface-modified PET films using various inorganic and biopolymer-based composites as active agents for the improvement of antimicrobial and barrier properties. Surface properties and antimicrobial activities of the developed films were investigated. Further, this project aims to develop a roll-to-roll coating process for applying active materials onto PET using the slot die coating technique. The primary objective is to optimize the coating parameters to achieve a stable and uniform film deposition on the PET substrate. This optimization process involves adjusting factors such as coating speed, slot die geometry, substrate temperature, and solution rheology to ensure consistent and reliable coating performance. Ultimately, the goal is to establish a robust manufacturing process capable of producing high-quality films for food packaging applications.

5.25 Title: Folding of Origami-based Multistable Laminates (Poster)

Authors: Ayan Haldar, Paul Weaver

Affiliation: University of Limerick

Abstract: With the recent advancement of additive manufacturing, bespoke manufacturing by design has enabled materials with highly anisotropic architecture. This has opened new avenues for realizing efficient shape morphing mechanisms in designing multifunctional structures attractive in a variety of engineering structures.

Structural origami is one such concept that utilizes sheet folding to facilitate low-dimensional structural systems spontaneously morphing into complex three-dimensional structures. Instead of relying on conventional morphing concepts involving many individual subunits, origami principles can create 3D shapes from a single sheet, depending on the crease folds and direction.

This project aims to design a continuous structure using fiber composite laminates, which are not pre-creased but can be folded at desired locations by employing hinge-like bistable mechanisms. Furthermore, we utilize Automated Tape Layup to design a variable stiffness morphing structure, particularly enabling us to address the often-conflicting requirements of load-carrying capability, shape adaptability, and lightweight construction.

5.26 Title: Optimization of 2-D Material Network Morphology by Liquid Interface Deposition (Poster)

Authors: Oran Cassidy, Emmet Coleman, Kevin Synnatschke, Jose Munuera, Jonathan Coleman
Affiliation: Trinity College Dublin

Abstract: 2-D materials have attracted considerable research interest in recent years, owing to their unique physical properties and relative material abundance that make them suitable for a wide area of applications. In particular, thin film networks of 2-D nanosheets are a promising candidate for realizing flexible electronic devices[1]. However, a major limitation of this application is the low carrier mobility observed in such nanosheet networks, which arises from the high inter-sheet junction resistance[2]. This work proposes to reduce junction resistance, and hence raise mobility, of these networks by optimizing the network morphology for conductive inter-sheet junctions, by use of a novel deposition technique which exploits the surface tension of immiscible fluid interfaces - Liquid Interface Deposition (LID).

[1] - Carey T et al. ACS Nano 2023, 17, 3, 2912–2922.
[2] - Kelly, A. G. et al. Nature Reviews Materials 2022, 7, 217–234.

5.27 Title: Fabrication of porous PTFE membranes (Poster)

Authors: E. Katoueizadeh, M.A. Morris

Affiliation: Trinity College Dublin

Abstract: Polymeric porous membranes are engineered structures with tailored pore sizes, shapes, and distribution. This presentation delves into the various methods employed to fabricate these membranes, highlighting techniques such as phase inversion, electrospinning, extrusion, pore forming agent, and track-etching. The selection of polymer materials, their

properties, and the impact on membrane performance will be also presented to explores the significance of controlling pore size and morphology in achieving desired separation and filtration outcomes. It touches upon the importance of membrane surface modifications for enhanced functionality and selectivity.

5.28 Title: Valorisation of wood residues into product (Poster)

Authors: M Masliha, J De Micco, M Troncoso Castellanos, Kevin O'Connor, Ramesh Babu

Affiliation: Trinity College Dublin

Abstract: This research project focuses on the valorisation of forest residues to create value-added materials, particularly emphasizing the production of next-generation wood materials. The primary objectives encompass extraction, characterization, valorisation and application of natural compounds from wood residues. Tannins, extracted from bark residues, underwent efficient extraction methods, including pressurized hot water extraction, ultrasonication-assisted extraction, and hydrodynamic cavitation-assisted extraction. Comprehensive analyses were employed to quantify and characterize the extracted tannins, leading to their separation and further analysis through various techniques [13C NMR, FTIR, and TGA].

The bulk extraction process involved the application of ultrasonication, followed by subsequent concentration through microfiltration, ultrafiltration, and forward osmosis techniques. The resultant concentrated tannin was then utilized on wood fibre samples.

Thereby, improving the properties of medium-density fibreboard [MDF] in terms of weatherability, and flame retardance. Furthermore, the tannin extracts evaluated as carbon source to produce biodegradable polymer polyhydroxyalkanoates [PHAs]. The bark, post-extraction, underwent enzymatic hydrolysis to ascertain the impact of extraction methods as a pre-treatment for enzymatic hydrolysis.

Another aspect involved utilizing industrial organosolv lignin for functionalization as a cationic flocculant for phosphate removal from wastewater streams. The adsorbent underwent thorough characterization using FTIR spectroscopy, SEM, EDS, TGA, zeta potential, and a point of zero charge measurement, and the study explored the adsorption mechanism, kinetics, and isotherm models.

This research contributes to the sustainable utilization of forest residues as a functional material and holds promise for developing environmentally friendly and economically viable materials

5.29 Title: Green polymer deposition opportunities in semiconductor industries: A Life cycle analysis prospective (Poster)

Authors: Eleanor Mullen and Professor Mick Morris

Affiliation: Trinity College Dublin

Abstract: Resource scarcity, increasing energy costs and environmental instability are major challenges to development in the semiconductor industry. Of the many subprocesses involved in the semiconductor industry lithography is particularly environmentally damaging. Lithography is used to pattern silicon wafers to produce integrated circuits (IC). As IC's become smaller, larger amounts of power and materials are required to pattern them. This increases ecosystem damage and puts strain on environmental resources. Improving sustainability in this industry is less costly and wasteful during the research and development stages of new lithographic techniques. This study uses Life Cycle Assessment (LCA) to compare emerging and conventional lithographic techniques in terms of environmental impact and technological readiness.

The emerging lithographic techniques this study focuses on are Area selective deposition (ASD) of polymer brushes and directed self-assembly (DSA) of block co-polymers (BCPs). ASD of polymer brushes facilitates selective deposition of a thin film over a select region of a substrate. DSA of BCPs allows for nanoscale patterning of a substrate and offers an alternative to techniques such as Extreme ultraviolet EUV lithography. These techniques present a novel opportunity for improving the sustainability of lithography by reducing the number of processing steps, energy and chemical waste products involved. LCA framework is applied here to assess the degree to which emerging lithographic techniques might be more sustainable than conventional lithography. This is central to verifying whether these new nanofabrication routes can replace conventional deposition techniques in the semiconductor industry as a more environmentally safe option. Studies of this nature will become imperative to the environmentally conscious development of science and technology.

5.30 Title: Extracting the temperature dependence of both nanowire resistivity and junction resistance from resistivity measurements on printed silver nanowire networks (Poster)

Authors: Emmet Coleman, Adam Kelly, Cian Gabbett, Luke Doolan, Shixin Liu, Neelam Yadav, Jagdish K. Vij, and Jonathan N. Coleman

Affiliation: Trinity College Dublin

Abstract: It has long been known that junctions play a vital role in the electrical performance of nanomaterial networks. Despite this, there are few methods to quantify the role of junctions in nanomaterial networks, which are often difficult or laborious. Additionally, there is currently no way of relating junction resistance to the conductivity of the overall network. This project aims to propose and verify an equation derived from a classical resistor chain model which relates the

junction resistance to the network conductivity for networks of 1D conducting materials. We then aim to use this equation to separate and extract values for the junction resistance (R_J) and DC nanowire conductivity (σ_NW) in silver nanowire networks. A nanowire length dependence study was carried out on AgNW networks and analysis of the DC network resistivity vs AgNW length displayed a linear response which allowed for the separation and extraction of R_J and σ_NW. Initial data suggests R_J=76±15Ω and σ_NW=7.8×10^7±2.4×10^7 S/m which is broadly in the expected range for AgNWs. Temperature dependence studies on these AgNW networks allowed for the monitoring of σ_NW and R_J as a function of temperature. Preliminary data suggests a linear response in R_J as a function of temperature and σ_NW behaves like a 1D metallic conductor across the measured temperature range, which further verifies the equation.

5.31 Title: Heterogeneous Fenton catalyst for the Oxidative Degradation of Low Density Polyethylene to Value-added Chemicals (Poster)

Authors: Rachel Breen, Justin D. Holmes, Gillian Collins

Affiliation: University College Cork

Abstract: As current recycling methods fail to tackle the increasing accumulation of plastic in our environment, chemical recycling of plastic waste offers an attractive solution to this global problem by converting waste polymers into high-value monomers. In contrast to other plastic polymers, polyethylene presents an enormous challenge due to its chemical inertness. Low density polyethylene has the highest primary waste generation of all plastics but one of the lowest recycling rates globally. Recycling efforts currently in place for polyolefins mainly involve high energy processes such as pyrolysis and hydrocracking. This work describes the design and synthesis of a heterogeneous Fenton-type catalyst for the oxidative degradation of LDPE. The process involves mild conditions under microwave irradiation resulting in oxidation and scission of the polyethylene chain to yield valuable mono- and dicarboxylic acids which can be used as feedstock chemicals for polymer production. The Fenton-type catalyst reported is an iron/ceria solid solution characterized by XRD, XPS, Raman Scattering, SEM, TEM and FTIR. The catalyst showed excellent activity at loadings as low as 1 wt. % as well as in a wide pH range and is recyclable over multiple cycles. Carboxylic acid products were identified and quantified using HPLC.

5.32 Title: Inversion of MoS2 Systems for Disorder Characterization (Poster)

Authors: Fábio Duarte, Shardul Mukim, Mauro Ferreira

Affiliation: Trinity College Dublin

Abstract: Inverse problems – problems in which we aim to obtain the causal factors of measurable effects – surround us in every field of research. Especially in condensed matter physics, the inversion of spectral signals is a particular inverse problem that has promising applications for material characterization and design. The solutions for inverse problems,

however, are usually elusive by nature, nonetheless, we propose an inversion methodology capable of tackling them. The work I am presenting reports how we have successfully applied this method to obtain structural information of, among other systems, vacancy-disordered MoS2 from its electrical conductivity signals with high accuracy on a theoretical level and also gathered qualitative information for vacancy characterization of real MoS2 systems from experimental transconductivity data, reinforcing the applicability of the proposed inversion method.

5.33 Title: LIGNIN PRE-TREATMENT AND DEPOLYMERIZATION FOR VALORIZATION INTO PRODUCTS (Poster)

Authors: J De Micco, M Troncoso Castellanos, F Cerrone, C Faulkner, K O' Connor, R Babu Padamati

Affiliation: Trinity College Dublin

Abstract: Lignin biomass offers many possibilities as feedstock for the chemical industry in replacing fossil-based resources thanks to its high abundancy, renewability, aromaticity, and biodegradability. The present work evaluates different pre-treatments and depolymerisation methods to achieve the best depolymerization performance with the lowest energy consumption to produce i) biodegradable polymer Polyhydroxyalkonate (PHA) by fermentation and ii) lignin-based polymer composites by melt mixing. Various technical lignins have been characterised using thermogravimetric-differential scanning calorimetric analysis, Fourier-transform infrared, and nuclear magnetic resonance spectroscopy. Both liquid and solid lignin depolymerised fractions were recovered and characterised. Preliminary results showed that the P.Putida KT2440 bacteria strain grows using the degraded lignin liquid fraction as carbon source. Depolymerised lignin solid fractions were used for composites preparation by melt mixing with commercial bio-polybutylene succinate (BioPBS). Composites prepared with degraded lignin showed improved thermal properties compared to virgin lignin composites.

5.34 Title: Piezoresistance and Conductivity in Graphene Nanosheet Networks (Poster)

Authors: Eoin Caffrey, Jose M. Munuera, Luke Doolan, Cian Gabbett, Tian Carey, Mark McCrystall, Alex McNamara, Joseph Neilson, Jonathan N. Coleman.

Affiliation: Trinity College Dublin

Abstract: Solution processed 2D nanosheet networks have found applications in printed transistors, batteries, photodetectors, catalysts and strain sensors. These networks are assembled from nanosheets in a liquid phase through a range of deposition techniques, yielding notably different structures. In this work, we prepared graphene inks by liquid phase (LPE) and electrochemical (EE) exfoliation with very different nanosheet aspect ratios (~30 vs ~1000) and processed them into networks via spray coating and liquid-liquid interfacial assembly techniques. Top-down SEM and FIB SEM 3D imaging of the networks show clear differences in morphologies due to both nanosheet aspect ratio and deposition technique. Small, rigid LPE nanosheets form

highly porous networks with point-like junctions, displaying different degrees of alignment depending on the deposition technique, while large, flexible EE nanosheets yield compact networks with large conformal junctions for every deposition technique. The electrical conductivities of these networks show a similar dependence on morphology, with a tenfold increase (~104 to ~105 S/m) for spray coated LPE and EE nanosheets. Piezoresistance measurements show a strong dependence on the network morphology on gauge factor, as predicted by the percolation-based model developed in previous work. Gauge factors of nanosheet networks were found to range between 0.4 and 350 depending on the network structure. This study casts light on the key tuning parameters to modify the network structure of nanosheet networks and the effect different structures have on the conductivity and piezoresistive response of the networks. Understanding these key electronic properties will pave pathways towards device applications using 2D materials, including strain sensors and printed flexible electronics."

5.35 Title: DESIGN AND FABRICATION OF LOW-LOSS HIGH-PERMEABILITY SOFT MAGNETIC MOULDABLE COMPOSITES FOR HIGH-FREQUENCY POWER INDUCTOR APPLICATIONS (Poster)

Authors: Sumit Sukhbasi Lal, Michael M. Morris, H. A. Baghbaderani, Liang Ye, Ranajit Sai, G. Wei, P. McCloskey

Affiliation: Trinity College Dublin

Abstract: Soft magnetic moldable composites (SM2Cs) would be ideal for the integration of inductors into circuits since they can be fabricated at a low temperature and pressure. However, most of the existing SM2Cs offer either low magnetic permeability (μ´) or quality factor (Q), especially at high frequencies (> 10 MHz). To address this issue, a bottom-up approach is reported from designing the composition of the magnetic filler, coating the filler with Polydimethylsiloxane (PDMS) brush, to the state-of-the-art casting process. This procedure gives rise to cores with an outstanding combination of μ´ and Q. The μ´ of our cores is 40% higher than the best available data at 10 and 25 MHz which is due to the high packing of cores. Our core also offers one of the highest Q at 10 MHz due to low hysteresis loss and low inter-particle eddy current loss as a result of the polymer brush insulating effect.

5.36 Title: Machine Learning Potentials for Flexible Metal-Organic Frameworks (Poster)

Authors: Abhishek Sharma and Stefano Sanvito

Affiliation: Trinity College Dublin

Abstract: Metal-organic frameworks (MOFs) are fascinating materials composed of organic linkers and inorganic metal clusters. MOFs with structural flexibility shows interesting properties such as opening and closing of molecular gates and lattice thermal expansion. To unravel the

molecular insights of flexibility in MOFs, molecular dynamics (MD) simulations are extremely useful. Accuracy of MD simulations depends on the employed force-fields. Generally used classical force-fields have limited accuracy compared to ab-initio quantum chemical methods such as density functional theory (DFT), however, the use of DFT is computationally very expansive. A common solution to these problems is given by machine learning potentials (MLPs), which combines the accuracy of DFT with the speed of classical force-fields.

In the present work, we considered the spectral neighbor analysis potential (SNAP), a class of linear atom-centered MLPs. We developed the SNAP potentials for two representative MOFs, namely ZIF-8 and MOF-5. Our MD results have shown successful predictions of the positive and negative thermal expansion of ZIF-8 and MOF-5, respectively, with an error of less than 1% on the lattice parameters as compared to experiments. We have also studied the vibrational density of states of both MOFs and found good comparison of predicted vibrational frequencies with the experimental infra-red and Raman spectrum frequencies. In addition to these, we have performed well-tempered metadynamics simulations to estimate the free energy barrier for the rotation of the phenylene ring in MOF-5. This calculation shows excellent agreement with the experimentally reported barrier for deuterated MOF-5. Our results show the accuracy of the developed SNAP and its potential as an alternative to classical force-fields for accurate computational investigation of future MOFs.

5.37 Title: Fluorinated Polyhydroxyalkanoates (FPHAs): Development, Characterization, and Applications (Poster)

Authors: Siva Ponnupandian, Meg Walsh, Kevin O'Connor, Ramesh Babu Padamati

Affiliation: Trinity College Dublin

Abstract: Poly(hydroxyalkanoates) (PHAs) represent a class of environmentally friendly, biodegradable, and biocompatible thermoplastics that are derived from bacterial sources. This work explores the development and characterisation of fluorinated polyhydroxyalkanoates (FPHAs). The Unsaturated PHA polymer was modified chemically via 'click chemistry' to introduce fluorinated side chains to understand the impact of the incorporation of fluorine on the PHA polymer properties. The fluorinated PHA polymer was characterised. FPHAs were used to prepare the polymer blends with various biodegradable polymers. Polymeric emulsions were also prepared using the chemically modified PHA polymer, and its properties were studied. The potential application of the emulsions as a coating material was analysed by coating the polymer over different fabrics. This research paves the way for further exploration of FPHAs by highlighting areas for improvement in fluorination levels and identifying potential applications in hydrophobicity-demanding sectors like textiles.

Reference:

(1) Dalton, B.; Bhagabati, P.; De Micco, J.; Padamati, R. B.; O'Connor, K. A review on biological synthesis of the biodegradable polymers polyhydroxyalkanoates and the development of multiple applications. Catalysts **2022**, 12 (3), 319.
(2) Babu, R. P.; O'Connor, K.; Seeram, R. Current progress on bio-based polymers and their future trends. Progress in biomaterials **2013**, 2, 1-16.
(3) Ebnesajjad, S. Introduction to fluoropolymers. In Applied Plastics Engineering Handbook, Elsevier, **2017**, 55-71.
(4) Kim, O.; Gross, R. A.; Hammar, W. J.; Newmark, R. A. Microbial synthesis of poly (β-hydroxyalkanoates) containing fluorinated side-chain substituents. Macromolecules **1996**, 29 (13), 4572-4581.

5.38 Title: Enhancing Electrochromism of Transition Metal Oxides using Fabry-Perot Interference (Poster)

Authors: Dilkhush Khicher, Evan Roy, Christopher Murray and David Mc CloskeyAffiliation:

Affiliation: Trinity College Dublin

Abstract: Electrochromic (EC) materials change their optical properties on the application of eternal bias. This change occurs due to ion intercalation and deintercalation which changes the EC material's oxidation state resulting in a strong change in colour and reflectivity(1). This change is reversible and hence these devices can be used in various applications such as smart windows(1), low energy display technologies(1) and tuneable strong absorbers.

The EC effect can be enhanced in thin films using multiple beam interference. In particular when we have a thin lossy dielectric material with a reflective metal backing, we observe broad absorption resonance known as zeroth Fabry Perot modes(2). When the thickness if the films is chosen correctly these modes can result in strong coloration in the visible range which is in very angle dependent. Combining this cavity design into EC devices can strongly enhance the colour and reflectivity change. This study shows the enhancement of colour and reflectivity of tungsten trioxide using hydrogen ion intercalation with a tungsten backing. With transparent conductive layers, the colour change goes from transparent to a dark blue, but on combining the zeroth order FP cavity more colours were observed depending on the thickness of WO3 layer.

References

[1] S., M.P.M., Mortimer, R.J., & Rosseinsky, D.R. (2007). Electrochromism and electrochromic devices. Cambridge, England: Cambridge University Press.
[2] Vaughan, M. (2017). The Fabry-Perot interferometer: History, theory, practice and applications. United Kingdom: CRC Press.

5.39 Title: Flexible polymer based wicking structures in heat pipes as part of modern prismatic cell-based battery thermal management systems (Poster)

Authors: David McCloskey & Simon Gynn

Affiliation: Trinity College Dublin

Abstract: The objective of this scoping project is to develop a prototype battery thermal management system (BTMS) on small scale to demonstrate that heat-pipes (HPs) can be utilized to provide superior thermal management than existing technologies. This would allow us to develop initial proof of concept data on a pouch-based HP which should enable further funding applications.

Recently, we have been researching flexible, light weight porous polymer based wicking structures in order to reduce the density and weight of HPs while maintaining their high thermal conductivity. Initial results indicate that this could be a viable BTMS for modern prismatic cell-based battery packs.

An emphasis by the Amber Centre is currently being placed on the development of innovative battery technologies, along with growth towards sustainable and collaborative research programmes. This project clearly aligns with Ambers current stated goals and will provide a valuable pool of knowledge in terms of modern BTMSs.

5.40 Title: Enhancing Electrochromism of Transition Metal Oxides using Fabry-Perot Interference (Poster)

Authors: Dilkhush Khicher, Evan Roy, Christopher Murray and David Mc Closkey

Affiliation: Trinity College Dublin

Abstract: Electrochromic (EC) materials change their optical properties on the application of eternal bias. This change occurs due to ion intercalation and deintercalation, changing the EC material's oxidation state. This change is reversible and hence these materials can be used in various applications such as smart windows, low energy display technologies, and tuneable strong absorbers.

The EC effect can be enhanced by thin film interference. In particular when we have a thin lossy dielectric on a reflective metal backing, we observe a resonances known as Fabry-Perot resonance cavity modes. Incorporating this cavity design with EC materials can strongly enhance their colour and reflectivity change therein.

This study focuses on showing the enhancement of colour and reflectivity change using tungsten trioxide and hydrogen ion intercalation with a tungsten backing. The results are then compared

to more conventional EC devices utilizing a transparent conductive backing layer such as ITO or FTO.

5.41 Title: Modifying the surface of Polymer Materials Used in the Fabrication of Plastic Bone Implants though the use of Block-copolymers. (Poster)

Authors: Jhonattan Frank Baez Vasquez, Michael A. Morris

Affiliation: Trinity College Dublin

Abstract: This study introduces an innovative approach to enhance the surface properties of high-performance polymers such as PEEK, CFPEEK, and UHMWPE, which are extensively utilized in a wide range of manufacturing applications. These materials boast excellent mechanical, chemical, thermal, and biocompatibility properties. However, their hydrophobic and chemically stable surfaces limit their use in areas such as catalysis, biointegration, and antimicrobial surfaces. Our methodology employs block copolymer lithography to fabricate metal oxide nanopillars on these polymers, aiming to achieve surface functionalization.

By utilizing a combination of solvent annealing and dip-coating techniques, we applied a thin layer of block copolymers, introduced metal ions, and used UV/ozone treatment to remove the polymer layer, leaving behind metal oxide nanopillars (Al2O3, Ag2O, MgO, CaO, TiO2)) with an average diameter of 20 nm, and effectively cover the polymer surfaces.

The modified surfaces were examined using atomic force microscopy (AFM), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS), confirming the correct formation and structure of the metal oxide layers. This method is efficient, cost-effective and potentially scalable, offering a significant advancement in enhancing the utility of polymers for applications such as medical implants, sensors, and electronics. This collaboration between the AMBER centre and Depuy Synthes Ireland presents a promising avenue for improving the performance of polymer-based implants.

5.42 Title: Optimizing Transparent Barrier Coatings for PET Beverage Packaging: Brush Polymer infiltration Approach (Poster)

Authors: Sherly Acosta, Michael A. Morris

Affiliation: Trinity College Dublin

Abstract: This project focuses on fabricating thin metal oxide layers on poly(ethylene terephthalate) (PET) substrates for beverage packaging. Utilizing a brush polymer infiltration method combined with a high energy oxidizing treatment, our aim is to create uniform and transparent barrier coatings, ensuring extended shelf life and mechanical strength of PET containers. Building on recent materials science advancements, we seek to align with PepsiCo's sustainability goals while enhancing gas permeation performance. The methodology is intended

to be adapted for moulded polymer surfaces, prioritizing transparency and mechanical properties. Optimization of the coating process will focus on beverage bottle surfaces, investigating parameters such as the metal source and brush removal treatments.

5.43 Title: The BioLaMer route to address food waste and petrochemical plastic challenges (Poster)

Authors: Sivakumar Krishnan, Michael A Morris, Sibu C Padmanabhan

Affiliation: Trinity College Dublin

Abstract: According to the Food and Agriculture Organization (FAO), one-third of food produced for human consumption is being lost or wasted. Composting, incineration and landfilling are the three major food waste management practices currently adopted. These processes are however not free from GHG emissions. Composting generates GHGs such as carbon dioxide (CO2) and nitrous oxide (N2O), while incineration produces CO2, water vapor, and various pollutants, depending on the composition of the waste. Although the CO2 generated from both these processes are generally considered as part of a natural carbon cycle, they are still responsible for a share of global warming. Landfilling is, however, the largest contributor of global warming amongst the three food waste management practices, emitting methane gas, which has 23 times or more global warming potential than CO2. This poster will showcase our European Innovation Council (EIC) Pathfinder Open project, BioLaMer, aimed at addressing two of the worlds pressing challenges such as food waste and petrochemical plastics challenge. BioLaMer seeks to demonstrate three mutually driving circular biorefinery concepts to address these challenges, thereby aligning with and supporting a number of European and global initiatives: Reducing GHG emissions, Complying with net-zero targets, Sustainable Development Goals and more. The BioLaMer project will impact the agri-food bioeconomy by supporting its transition to an environment, economic and socially sustainable one, thus, aiming to leave the earth a better place to live for the future generations to come.