6th Annual Inter CDT Conference 2025

Cambridge

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Participating CDTs

- Formulation Engineering CDT – University of Birmingham
- Soft Matter for Formulation and Industrial Innovation CDT – Durham University, University of Leeds and the University of Edinburgh
- Nanoscience and Nanotechnology CDT – University of Cambridge
- Molecules to Products CDT – University of Leeds
- Topological Design CDT – University of Birmingham
- Engineered Tissues for Discovery, Industry and Medicine CDT (LifETIME) – Aston University, University of Birmingham and the University of Glasgow
- Sensor Technologies and Applications in an Uncertain World (Sensors CDT) - University of Cambridge

Introduction

We are delighted to welcome you to the 6th Annual InterCDT Conference - a student-led tradition that brings together doctoral researchers from Centres for Doctoral Training (CDTs) across the UK. Following the success of last year's conference in Durham, we are thrilled to host you in the historic and inspiring city of Cambridge for 2025.

This conference is uniquely run by students, for students, fostering a vibrant, inclusive, and collaborative atmosphere. It offers a valuable opportunity for doctoral researchers to share their work, explore new perspectives across disciplines, and build connections that could shape the future of science, technology, and innovation. Over the coming days, we look forward to engaging discussions, cutting-edge research, and cross-disciplinary exchange.

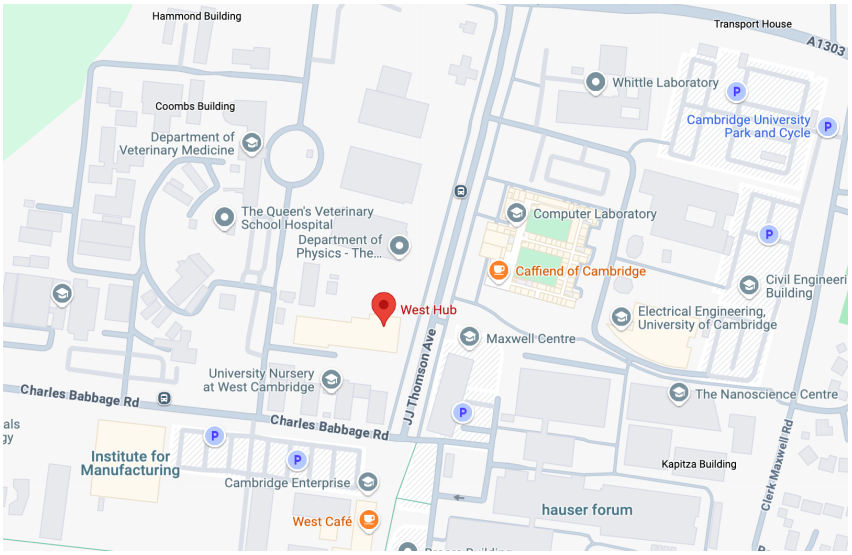
We are deeply grateful to our generous sponsors - the, NanoCDT, Sensor CDT, Formulation CDT, West Hub Small Grants Programme, Churchill College, the Royal Society of Chemistry, and the Biochemical Society - whose support has made this event possible. Their contributions help nurture collaboration and professional growth among the next generation of scientists and innovators.

Thank you for joining us in Cambridge. We look forward to learning from your work, celebrating your achievements, and building lasting connections. Here's to a fantastic conference ahead!

Celia Chen, Laurence Brazel & Reece McCoy
NanoDTC

Getting here

The conference will be held at the **West Hub, JJ Thomson Ave, Cambridge, CB3 0US, at the University of Cambridge**.



By train/bus

The closest train station is Cambridge Station.

There is a bus stop outside the station for West Cambridge site. You can take the:

- U1/U2 Universal towards Girton Corner or Eddington. Alight at the West Hub stop. Discounts may be available upon showing a student ID.
- X3 Hunting bus station. Alight at Cam Uni Vet School and walk 6 minutes to West Hub.

By train/taxi

There is also a taxi rank outside the train station and Uber is available. A taxi ride from Cambridge station to West Hub is approximately 7 minutes and will cost £9-11.

By car

There is a Park and Ride Carpark on Madingley Road which is a 15 minute walk to West Hub. This is free for up to 18 hours of parking and anything beyond this is charged. Further information can be found here: https://cambridgeparkandride.info/madingleyroad-about.shtml

Accessibility

If there is anything we can do to help with accessibility requirements please feel free to reach out to us!

Getting to the conference dinner

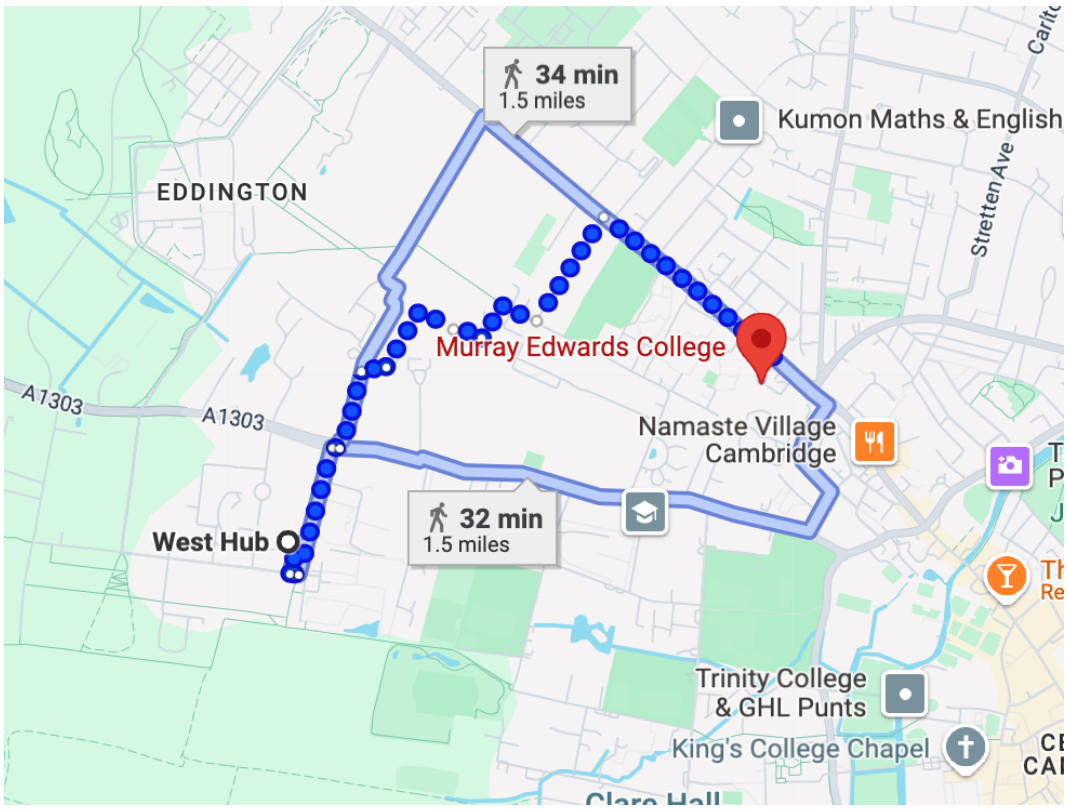
The Conference dinner on the 26th of June, starting at 7:00 pm at Murray Edwards College in the Fellows Suite. It is recommended that attendees check into their accommodation between the poster session and the conference dinner. Please do check the distance between West Hub, your accommodation, and Murray Edwards College and plan accordingly.

Getting there on foot

The walk from West Hub to Murray Edwards College will take approximately 30 minutes.

Getting there by taxi

The taxi/Uber ride from West Hub to Murray Edwards College will take approximately 6 minutes and will cost £8-11.



Presenter information

Oral presentations

Please bring with you a copy of your presentation on a USB stick to upload to the session room computer. The session chair will arrange for speakers to transfer presentations in advance of the session – it helps if you can put your name in the file name.

The Chair session will keep track of time and lead the Q&A session.

The time limits for the oral presentations are:

- Short oral presentation: 5 minutes with no questions
- Long oral presentation: 15 minutes + 5 minutes presentation

Poster presentations

Please print your poster in A0 size and pin the poster up on the boards before the poster session. You will be able to do this anytime throughout the day – but doing it upon arrival is preferred/

We may be taking photos during the conference, please let us know if you don't want your photo to be taken or uploaded on media platforms.

6th Annual Inter CDT Conference 2025
26 – 27th June 2025
University of Cambridge

Day 1: 26th of June 2025

9:30 am – 10:00 am	Registration	
10:00 am – 11:00 am	Icebreaker session	
11:00 am – 12:35 pm	**Session 1** **Chair: Juliana Ferraro**	
11:00 am – 11:20 am	Lizzie Evans	S = ½ Kagome Magnets in the Two-Dimensional Limit
11:20 am – 11:40 am	John Cooper	Fusion Reactors HATE This One WEIRD Trick!!!!
11:40 am – 11:45 am	Safiyah Hussain	Investigation of Oxidation Behaviour and Passivation Rates for Recycled Hydrogen Processed NdFeB Powder
11:45 am – 12:05 pm	Khizra Abdul Wadood	Leveraging Powder Characterisation to Predict Dissolution in Pharmaceutical Formulations
12:05 pm – 12:10 pm	Vinothan Vaheesan	Tunable Topological Metasurface with Leaky-wave Features
12:10 pm – 12:30 pm	Will Ogle	Synthesis and characterisation of liquid crystals bearing a novel uracil derived headgroup.
12:30 pm – 12:35 pm	Charlie Brayson	Enhancing a Novel Carbon Capture Technology Using Open-Source CFD Modelling
12:35 pm – 1:50 pm	Lunch	
1:50 pm – 2:40 pm	**Session 2** **Chair: Larry Brazel**	
1:50 pm – 2:10 pm	Hazal Sezer	Exploring the internal dynamics of resonant acoustic mixing using positron emission particle tracking
2:10 pm – 2:15 pm	Emily Maxwell	DNA Hydrogels for Stem Cell Engineering
2:15 pm – 2:20 pm	Natalie Richards	Bacterial Motility and Membrane Deformation in Biohybrid Vesicles
2:20 pm – 2:40 pm	Joseph McHale	Improving Supersaturation Control in Low-Solubility Systems: Integrating Machine Learning with Model Predictive Control
2:40 pm – 3:40 pm	**Keynote speaker** *Plastics: A Wicked Problem* Dr Claire Barlow	
3:40 pm- 5:30 pm	**Poster session**	
5:30 pm – 7:00 pm	Check into hotel and get ready for conference dinner	
7:00 pm – 10:00 pm	Conference dinner at Murray Edwards College	

Day 2: 27th of June 2025

9:30 am – 10:20 am	**Session 3 Chair: Reece McCoy**	
9:30 am – 9:50 am	Saathana Ambikaibalan	Impact of plant-based wax crystal structure and morphology on physical property and stability of oleogels
9:50 am – 9:55 am	Aran Klair	Evolutionary Optimisation of a Pharmaceutical Feeder System
9:55 am – 10:15 am	Tara Murphy	Bayesian Optimization for Automatic Tuning of Sensor Dots in Silicon Quantum Dot Arrays
10:15 am – 10:20 am	Charlie Gardner	Strip Casting of SmCo Alloys to Reduce Manufacture Costs of Sm2(Co,Fe,Zr,Cu)17 Permanent Magnets
10:20 am – 11:20 am	**Panel discussion: From CDT to Industry – Insights** Dr Jeroen Verheyen – Semarion Dr Tobias Naegele – Technology Consultant at TTP Plc. Formerly NanoDTC Dr Sophie Oldroyd – Patent Lawyer at Carpmaels & Ransford. Formerly Sensors CDT	
11:20 am – 11:50 am	**Tea Break**	
11:50 am – 1:10 pm	**Session 4 Chair: Vinothan Vaheesan**	
11:50 am – 12:10 pm	Benjamin Devenish	From Tip to Ship: Characterisation of New Marine Antifouling Coatings After Aging
12:10 pm – 12:30 pm	Eleonora De Giorgi	Optimising PAT for Continuous Direct Compression using a Feed Frame Simulator
12:30 pm – 12:50 pm	Lucie Hlubinková	Nanomechanical measurements of solid fabric enhancer (SFE)
12:50 pm – 1:10 pm	Sarah Ferris	Characterisation of iron oxides in red gypsum using TEM: Towards valorisation of TiO_2 co-products

1:10 pm – 2:10 pm	**Lunch Break**	
2:10 pm – 3:00 pm	**Session 5 Chair: Celia Chen**	
2:10 pm – 2:30 pm	Larry Brazel	Exploring Discharge Product Distribution in Li-O2 Batteries
2:30 pm – 2:35 pm	Jieni Wang	Using iPSC-derived Motor Neuron as a model to investigate the pathological effect of mutant Fused in Sarcoma (FUS) on the cellular calcium and organelle dynamics in Amyotrophic Lateral Sclerosis (ALS)
2:35 pm – 2:40 pm	Supreeth Sundar	Liquid Foams in Motion: Probing Multiscale Rearrangements with Adhesion Tensiometry
2:40 pm – 3:00 pm	Gerda Luht	Physicochemical Characterization of Asphaltenes Partitioned at Oil-Water Interfaces
3:00 pm – 3:30 pm	**Tea Break**	
3:30 pm – 4:05 pm	**Session 6: James Robert Austin**	
3:30 pm – 3:50 pm	Ella Sapsford	Tough meets Stretchy: towards systematic control of threaded y-CD for slide-ring materials
3:50 pm – 3:55 pm	Harvey Smart	Synthesis and analysis of transition metal pyrithiones and pyridineselenones to address antimicrobial resistance
3:55 pm – 4:00 pm	Dylan Cuskelly	Forging Fusion-Grade Steels in the 3D Printer: The Power of In-Situ Control
4:00 pm – 4:05 pm	Harshita Dani	Enhancing the Penetration of Cosmetic Actives into the Skin
4:05 pm – 4:25 pm	Award judging	
4:25 pm – 4:40 pm	Award ceremony and closing remarks	

Poster session

P1	James Austin	Deformation relaxation dynamics in dioxaborolane vitrimers
P2	Caitlin O'Brien	High Refractive Index Liquid Crystal Molecules
P3	Harry Jones	Reengineering PLFs: Molecular Upcycling
P4	Thanmaya Arunkumar	Development of sustainable hair conditioning technologies
P5	Jacob Bracegirdle-Morais	Novel Characterisation of Topographically Complex Metal Additively Manufactured Implant Surfaces
P6	Safiyah Hussain	Investigation of Oxidation Behaviour and Passivation Rates for Recycled Hydrogen Processed NdFeB Powder
P7	Emily Maxwell	DNA Hydrogels for Stem Cell Engineering
P8	Charlie Brayson	Enhancing a Novel Carbon Capture Technology Using Open-Source CFD Modelling
P9	Natalie Richards	Bacterial Motility and Membrane Deformation in Biohybrid Vesicles
P10	Aran Klair	Evolutionary Optimisation of a Pharmaceutical Feeder System
P11	Harshita Dani	Enhancing the Penetration of Cosmetic Actives into the Skin
P12	Harvey Smart	Synthesis and analysis of transition metal pyrithiones and pyridineselenones to address antimicrobial resistance
P13	Dylan Cuskelly	Forging Fusion-Grade Steels in the 3D Printer: The Power of In-Situ Control
P14	Lizzie Evans	S = ½ Kagome Magnets in the Two-Dimensional Limit
P15	Khizra Abdul Wadood	Leveraging Powder Characterisation to Predict Dissolution in Pharmaceutical Formulations
P16	Gerda Luht	Physicochemical Characterization of Asphaltenes Partitioned at Oil-Water Interfaces
P17	Hazal Sezer	Exploring the internal dynamics of resonant acoustic mixing using positron emission particle tracking
P18	Joseph McHale	Improving Supersaturation Control in Low-Solubility Systems: Integrating Machine Learning with Model Predictive Control
P19	Eleonora De Giorgi	Optimising PAT for Continuous Direct Compression using a Feed Frame Simulator
P20	Lucie Hlubinková	Nanomechanical measurements of solid fabric enhancer (SFE)
P21	Larry Brazel	Exploring Discharge Product Distribution in Li-O2 Batteries
P22	Ella Sapsford	Tough meets Stretchy: towards systematic control of threaded y-CD for slide-ring materials
P23	Tara Murphy	Bayesian Optimization for Automatic Tuning of Sensor Dots in Silicon Quantum Dot Arrays
P24	Victoria Byelova	A mesoscale approach to dynamic protein unfolding during gel network formation
P25	Adrian Ho	PD-L1 Nanoparticle Protein Degrader for targeting Chemotherapy-Induced Senescence
P26	Isabella Teck	High Performance Resistive Switching Devices for Sustainable Artificial Intelligence based on YSZ thin films
P27	Aldric Goh	Probing the electrical characteristics of passivated InAs nanowires using terahertz time-domain spectroscopy
P28	Viola Huf	3D Printed Liquid Crystal Elastomers
P29	Edward Saunders	Electrical impedence spectroscopy for flow battery electrode engineering
P30	Timothy Lambden	Investigating local chain orientation in conjugated polymers
P31	Tolu Agoro	Characterisation of hot carrier effects in ultra-thin solar cells
P32	Juliana Ferraro	Lights, Camera, Droplets! Platform development to study impact behaviour on a pleural tissue phantom

Keynote Lecture

Plastics: A Wicked Problem

Dr Claire Barlow
Emeritus Faculty, Cambridge University Engineering Department

Artificial plastics have infiltrated the market as a result of their low cost, low weight, manufacturability and versatility deriving from their wide range of useful mechanical and physical properties. Plastics have been transformational and we now rely on them in all aspects of our lives. However, one of their most desirable attributes, their durability, is now threatening their downfall: what we do with plastics when they become rubbish at end-of-life is a real problem and a huge amount ends up littering the environment. Public outrage can lead to ill-considered 'Ban plastic' reactions which can have undesirable environmental and social consequences. We need to think in terms of whole lifecycle systems rather than tackling one just aspect of this complex issue.

We must take action to solve the problem of existing and future plastic waste. But plastics still need to be part of our lives. Can we find ways to build end-of-life design into plastics and plastic products? Can we use them more wisely? What potential is there for using other materials rather than plastics for particular applications? We will explore some ideas and try to look for balanced approaches to the future of plastics.

Claire Barlow did her undergraduate degree and PhD at Cambridge before taking up a lectureship in the Engineering Department. She held a series of leadership roles, first as Course Director for the Manufacturing Engineering Tripos, then successively in the Engineering Department Director of Undergraduate Education, Deputy Head (in charge of teaching) and Interim Head of Department. She is now Emeritus Faculty, and Fellow Emerita of Newnham College.

Her early research used electron microscopy to understand the relationships between microstructures and mechanical properties, initially in metals but broadening out into other materials over time. She then became interested in environmental aspects of production, use and disposal of engineering materials, with a focus on mechanical and physical properties of recycled materials. She has worked on technical projects developing end-of-life treatments for a range of materials including natural materials, paper and aluminium. The problems of managing waste materials are integrally connected with wider industrial, social and political issues, and her work includes studies of waste management in international settings.

Investigation of Oxidation Behaviour and Passivation Rates for Recycled Hydrogen Processed NdFeB Powder

[1]Hussain, Safiyah, [1]Nayebossadri, Shahrouz, [1]Kozak, Viktoria, [1]Brooks, Oliver, [1]Walton, Allan

[1] University of Birmingham, Edgbaston, Birmingham, B15 2TT

Due to their exemplary magnetic properties and versatility, neodymium magnets (Nd2Fe14B) are the most widely employed rare-earth (RE) magnets. RE elements are high on the EU critical materials list for supply risk due to instability within the rare earth element global supply chain, and demand is projected to continue increasing [1]. There is a growing focus on establishment of alternative neodymium supply. A possible solution is recycling of large reserves of spent NdFeB magnets, reducing demand for virgin material, and providing a more sustainable future supply.

The HPMS recycling method patented at the University of Birmingham uses hydrogen to extract demagnetised NdFeB powder from magnets contained within scrap sources. The fine hydrogenated powder produced by HPMS is highly pyrophoric and susceptible to oxidation during subsequent processing. The oxidation behaviour and stability of the powder has implications on the viability of the downstream processing.

This work investigates the oxidation behaviour of recycled magnetic material produced from the HPMS process. Powders were analysed from multiple stages in the HPMS process, using oxidation under thermogravimetric analysis.

References

[1] Blengini, G.A., El Latunussa, C...*et al*. European Commission

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Fusion Reactors HATE This One WEIRD Trick!!!!

[1]Cooper, John, [1]Carrington, Matthew, [1]Wang, Yiqiang, Cai, Biao*

[1] United Kingdom Atomic Energy Authority, Culham Centre for Fusion Energy, Culham Science Centre, Abingdon OX14 3EB
*School of Metallurgy and Materials, University of Birmingham, Birmingham B15 2TT, UK

Fusion energy presents an immense opportunity to provide limitless clean energy, but it still faces significant challenges before it becomes a commercially viable energy source. Chief among these is developing materials that can withstand the intense temperatures, plasma damage, and neutron bombardment within the reactor, without releasing impurities, trapping fuel, or otherwise disrupting the fickle plasma that sustains the fusion reaction [1]. W-Cu composites have been identified as a candidate material for heat sink components in fusion reactors, but it is not yet well understood how they deform, crack, and fail in fusion relevant scenarios. This work uses optical and electron microscopy, and X-ray and neutron diffraction to characterise W-Cu composites in situ during tensile loading to reveal the contribution of the individual phases to the mechanical properties of the composite as a whole.

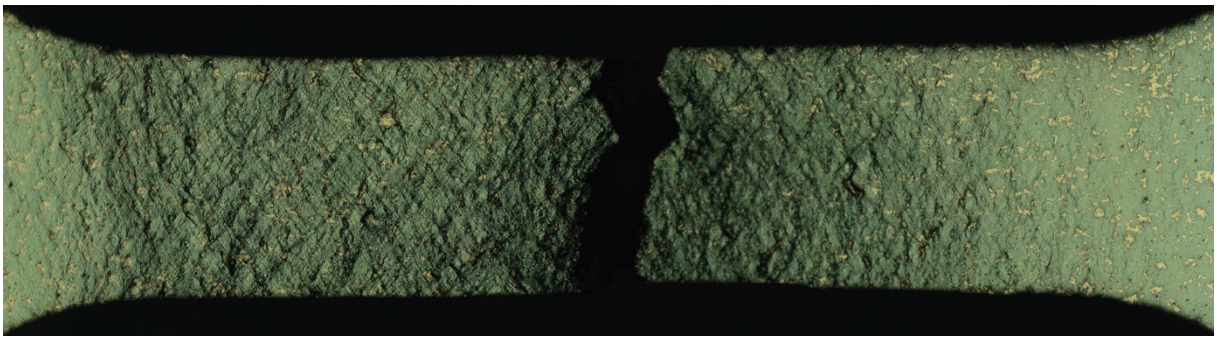

Figure 1: Fractured surface of W-Cu composite sample, imaged with optical microscopy.

Acknowledgements: The UK-EPSRC Centre for Doctoral Training in Topological Design and the United Kingdom Atomic Energy Authority.

References

[1] Knaster, J., Moeslang, A. & Muroga, T. Nature Phys (2016) 12, 424-434

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S = ½ Kagome Magnets in the Two-Dimensional Limit

[1]Evans, Lizzie, [1]Dolling, Tristan, [1]Pitcairn, Jem, [1]Costantini, Giovanni, Clark, Lucy*

[1] School of Chemistry, University of Birmingham, Edgbaston, Birmingham, UK
*School of Chemistry, University of Birmingham, Edgbaston, Birmingham, UK

Since the discovery of intrinsic ferromagnetism in two-dimensional (2D) layers of CrI_3 and $Cr_2Ge_2Te_6$ in 2017. [1,2] There has been growing interest in 2D magnetic materials. Their low dimensionality gives them the potential to host exotic magnetic behaviour, which could be harnessed for applications in quantum computing. [3] Magnetic metal-organic nanosheets (MONs) are a class of two-dimensional materials which are highly tuneable, [4] giving them distinct advantages over purely inorganic magnets. They can be obtained through the top-down exfoliation of layered metal-organic frameworks (MOFs), which overcomes the weak van der Waals (vdW) forces between the layers to separate them. As such, they provide a route to new 2D magnets that are stable in the monolayer limit. Following the Nobel-prize winning discovery of graphene,[5] the Scotch tape method has been widely used to exfoliate inorganic vdW materials, but has only been applied to layered MOFs in a handful of cases. [6,7] In this talk, I will highlight our recent advances in the Scotch tape exfoliation of a layered kagome magnet, MOF-bipy, and our characterisation of this material both in bulk, and on approaching the 2D limit.

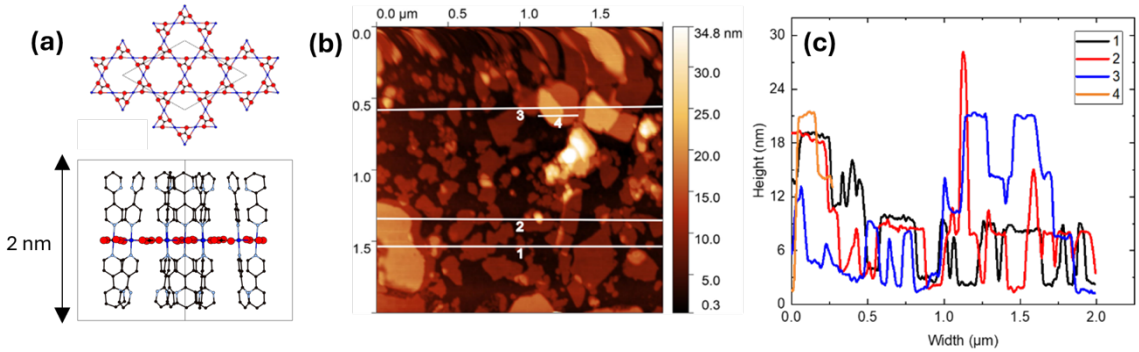

Figure 1: (a) Crystal structure of MOF-bipy viewed in the ab-plane (top) and along the c-axis (bottom). Space group P3. Cu, dark blue; O, red; C, black; N, light blue. Charge-balancing perchlorate anions are omitted from the hexagonal channel for clarity. AFM topographical image (b) of MOF-bipy nanosheets obtained through mechanical exfoliation using the Scotch tape method. AFM profiles (c) indicate nanosheet heights and lateral dimensions; nanosheets of height - 6 nm (three layers) are seen across the silicon substrate with uniform coverage.

Acknowledgements: I would like to thank the STFC for beamtime access and the EPSRC for their support through the following grants: EP/S02297X/1 (CDT Topological Design), EP/T02271X/1 (A New Paradigm for Quantum Materials Discovery) and EP/V028774/1 (Midlands Mag-Lab).

References

[1] B. Huang et al., Nature, 2017, 546, 270-273.
[2] C. Gong et al., Nature, 2017, 546, 265-269.
[3] B. Keimer and J. E. Moore, Nat. Phys., 2017, 13, 1045-1055.
[4] D. J. Ashworth and J. A. Foster, J. Mater. Chem. A, 2018, 6, 16292-16307.
[5] K. S. Novoselov et al., Science, 2004, 306, 666-669.
[6] Alexandre Abherv et al., Chem. Sci., 2015, 6, 4665.
[7] Madison E. Logelin et al., Chem. Sci., 2024, 15, 15198.

Leveraging Powder Characterisation to Predict Dissolution in Pharmaceutical Formulations

[1,2]Abdul Wadood, Khizra, [2]Molloy, Matthew, [1]Windows-Yule, Christopher, [1]Ingram, Andy

[1] School of Chemical Engineering, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK
[2] Oral Product Development, Pharmaceutical Technology and Development, Operations, AstraZeneca, Macclesfield, SK10 2NA, UK

Understanding the dissolution and dispersion of pharmaceutical powders is vital for drug efficacy, patient compliance, and manufacturing efficiency. However, predicting these behaviours is challenging because different powders exhibit unique flow properties that influence dissolution stages such as wetting, sinking, swelling, and dispersion. This study characterises pharmaceutical excipients by measuring particle size distribution, flowability, wettability, and cohesion, linking these attributes to the progression of dissolution phenomena. Controlled experiments elucidate how powder flow impacts dissolution rate and extent. A data-driven framework, employing machine and deep learning algorithms, is developed to predict dissolution behaviour from powder characteristics, thereby reducing the need for extensive experimental trials. This integrated approach streamlines formulation development, accelerates process scale-up, and improves the reliability of product performance predictions.

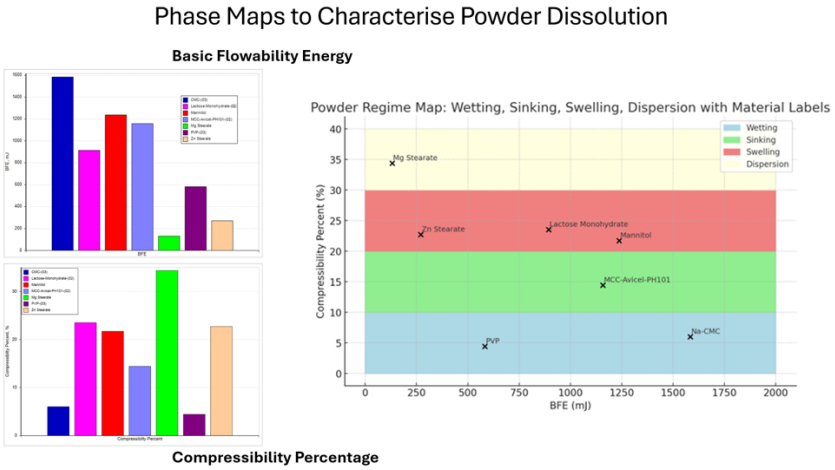

Figure 1: Phase map to characterise powder dissolution regimes

Acknowledgements: The lead author is studying for an Engineering Doctorate (EngD) at the University of Birmingham, and acknowledges funding received from the Centre for Doctoral Training in Formulation Engineering via the Engineering and Physical Sciences Research Council and AstraZeneca. EPSRC Grant: EP/S023070/1

Tunable Topological Metasurface with Leaky-wave Features

[1]Vaheesan, Vinothan, [1]Mitchell, Kevin, [1]Trussler, Daniel, [2]Navarro-C.A, Miguel, Feresidis, Alexandros[1,*]

[1] QinetiQ Group plc, Farnborough, United Kingdom
[2] University of Birmingham, School of Physics and Astronomy, Birmingham, United Kingdom

This paper proposes a novel mode-tuning mechanism in a photonic topological metasurface to switch between a weakly/non-radiating guided surface line wave function and a highly directive leaky wave antenna function. We investigate the edge modes shifting in the supercell dispersion diagrams under different configurations. We conduct full structure simulations at 18 GHz and monitor the waveguiding and radiation. The guided wave variation showed a radiation efficiency of 5.94 % and a semi-isotopic radiation pattern, whilst the leaky wave antenna variation showed a highly directive beam with a peak directivity of 12.42 dB. We were able to show, at 18 GHz, a gain difference of 15.40 dB between the two configurations.

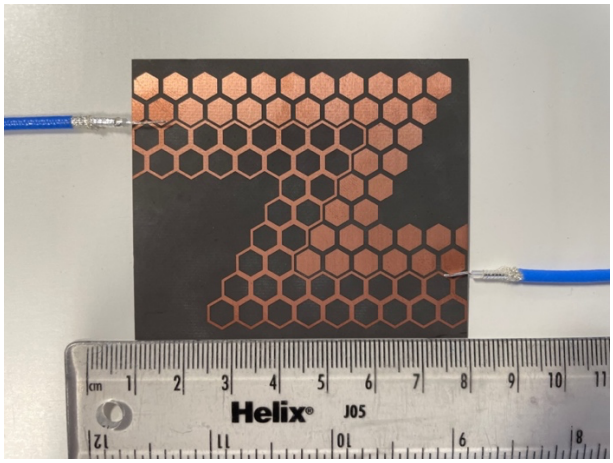

Figure 1: Fabricated photonic topological metasurface with a zigzag interface. Coaxial cables used to measure the tranmission properties.

Acknowledgements: This work was funded by QinetiQ Group plc and the University of Birmingham and the research falls under the UK Engineering and Physical Sciences Research Council Grant number EP/S02297X/1.

References

[1] T. S. Rappaport, Y. Xing et al., “Wireless communications and applications above 100 ghz: Opportunities and challenges for 6g and beyond,” IEEE access, 2019, vol. 7, pp. 78 729–78 757.
[2] D. J. Bisharat and D. F. Sievenpiper, “Electromagnetic-dual metasurfaces for topological states along a 1d interface,” Laser & Photonics Reviews, 2019, vol. 13, no. 10, p. 1900126.

Synthesis and characterisation of liquid crystals bearing a novel uracil-derived headgroup.

[1]Ogle, William, [1]Baker, Daniel, [1]Ries, Michael, [1]Mandle, Richard

[1] School of Physics and Astronomy, University of Leeds, LS2 9JT

Some molecules display a mesophase between their crystalline solid state and isotropic liquid state. These are known as liquid crystals (LCs), which have extensive applications in display technology, and were fundamental to the digital revolution. Long rod-shaped liquid crystals, whose behaviour is temperature dependent, are known as calamitic thermotropic liquid crystals. These are typically all derived from petrol chemicals, with less than 3% liquid crystal having any reference to sustainable chemistry or its practises.
Uracil is a functionalised pyrimidine ring and is one of the four nucleotide bases found in RNA. Uracil has successfully been extracted from nature for over two centuries,[1,2] with synthetic routes from urea, 2,4-dimethoxypyrimidine, and deamination of cytosine also being possible. [2-4]
Herein, liquid crystalline materials bearing a novel uracil motif have been synthesised. Phases such as: the conventional nematic; used in display technology, the chiral nematic; used in sensing applications.

Acknowledgements: Calum Gibb, Jordan Hobbs, Stuart Berrow

References

1 Irene. M. Lagoja, Chem Biodivers, 2005, 2, 145.
2 D. Davidson and O. Baudisch, J Am Chem Soc, 1926, 48, 2253-492.
3 D. Ramesh, B. G. Vijayakumar and T. Kannan, Eur J Med Chem, 2020, 207, 112801.
4 R. J. De Pasquale, Ind. Eng. Chem. Prod. Res. Dev, 1978, 17, 278.

Physicochemical Characterization of Asphaltenes Partitioned at Oil-Water Interfaces

Gerda Luht[1], Van Kelly[2], David Clarke[2], Sven Schroeder[1], Andy Ross[1], Deepak J Mukkattukavil[1], Tom Robinson[3], Peter J Dowding[3], David Harbottle[1]

[1] School of Chemical and Process Engineering, University of Leeds; 2. School of Chemistry, University of Edinburgh; 3. Infineum UK Ltd., Oxfordshire

Asphaltenes are high molecular weight, polyaromatic compounds defined as a solubility class of crude oil, soluble in aromatic solvents and insoluble in aliphatic solvents. This broad definition has hindered progress in treating issues like emulsion stabilisation and deposition. New insights into problematic asphaltene properties have developed through fractionation into interfacially active and non-partitioning asphaltenes. The strongly interfacially active fraction is typically ~2 wt% of the total asphaltenes, with higher heteroatom content, and some studies suggesting higher aliphaticity; both characteristics promoting strong adsorption at solid-liquid and liquid-liquid interfaces (1,2).

The presentation will show how, with application of a sequential extraction method, up to 15 wt% of interfacially active asphaltenes has been extracted. Each individual sub-fraction was extensively characterized (elemental analysis; FTIR; FTICR MS; XPS; interfacial tension; QCM) to elucidate changes in the physicochemical properties of the sub-fractions with each sequential extraction. After the first few extractions, the characteristic properties of the interfacially active asphaltenes become less distinct, gradually transitioning towards non-partitioning asphaltenes. This shift strongly aligns with changes in asphaltenes adsorption, providing a clearer understanding of the key structural and chemical properties governing asphaltene adsorption behaviour. These new insights are increasing understanding of environment-dependent asphaltene behaviour beyond the solubility class definition.

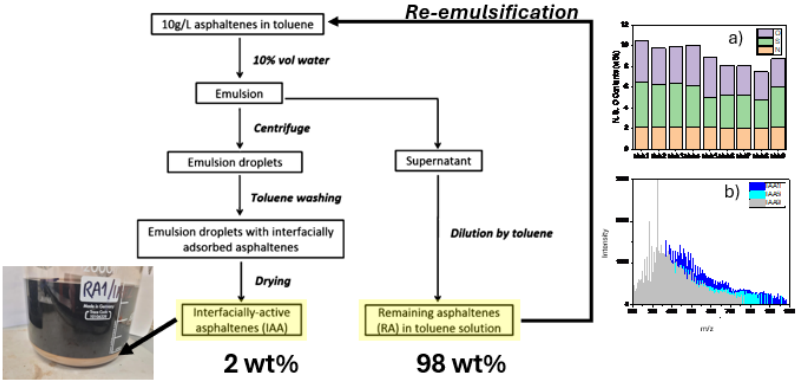

Figure 1: Workflow to sequentially extract the most interfacially active asphaltenes (IAA1-9) from the remaining asphaltenes (RA1-9). Shifts in heteroatom content (a) and molecular weight distributions (b).

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DNA Hydrogels for Stem Cell Engineering

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Biomimicry is vital for the enhanced function and biocompatibility of biomaterials. Hydrogels offer a promising solution to many of the problems tissue engineering aims to solve, such as tissue repair, modelling, and drug delivery. Tuneable biomaterials are commonly used in tissue engineering as controlling properties allows for driving specific stem cell differentiation. DNA's unique complementary base pair binding, environmental sensitivity and response, shear thinning properties and multifunctionality make it an incredible 'smart'™ material and potential bioink. Few DNA hydrogels have been developed exploiting its different properties. Often DNA is used as crosslinkers for a polymer-based gel, failing to utilise other DNA specific characteristics such as custom strand design. Other techniques such as rolling circle amplification and hybridisation reactions have resulted in some interesting gels, but these techniques do not allow for a true DNA based bioink where immediate crosslinking is required. We will engineer a stem cell laden DNA hydrogel system - investigating printability and biocompatibility with high spatial organisation and desirable mechanical properties.

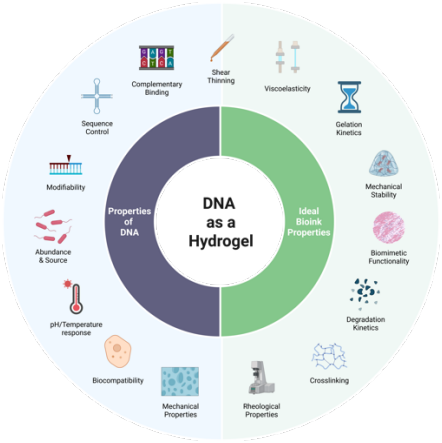

Figure 1: DNA hydrogels have many desirable properties in tissue engineering that additionally align with ideal bioink properties as shown in the figure.

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Exploring the internal dynamics of resonant acoustic mixing using positron emission particle tracking

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Blending composites like syntactics and resin-based systems conventionally occur through extended mixing in rotary drums or traditional blade-based mixers. After the blending process, the mixture is poured, molded into blocks, and subjected to subtractive machining. These procedures are time-intensive, generate waste, and pose potential hazards, especially when dealing with materials sensitive to energy. To address these challenges, we have explored the application of Resonant Acoustic Mixing (RAM), an innovative technology for blending powder/powder, powder/fluid, and fluid/fluid mixtures. So far, we have studied the two most fundamental variable parameters in RAM mixing – the fill height of the vessel and the strength with which it is vibrated. To test how the fill level and the vibrational acceleration to which it is exposed affect mixing efficiency, we have performed a design of experiments imaging a simple material, microcrystalline cellulose (MCC) within a RAM mixer using positron emission particle tracking (PEPT).

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High Refractive Index Liquid Crystal Molecules

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High refractive index liquid crystal materials have found to be favourable in a wide range of applications such as liquid crystal displays and communication devices. Having an increased refractive index allows for thinner devices. Development of increasingly higher refractive index materials stems from continuous demand for ever smaller optical components with increasing performance, for example within AR/VR. A significant challenge relates to the absorption of visible light (leading to yellow colouration) or UV light (leading to poor stability). The challenge therefore is to find ways to decouple absorption from high refractive index through molecular structure, with the aim of producing high performing materials without the drawbacks associated with incumbent systems. Improvement of refractive index can be achieved via increased electron density through exploiting conjugation as well as the incorporation of heavier, more polarisable atoms. In this work I compare the effect of different conjugated systems: naphthyl, biphenyl, and 2-phenylnaphthyl groups, and an alkyne bond - on various properties, e.g. transition temperatures, UV-Vis absorption, and optical anisotropy.

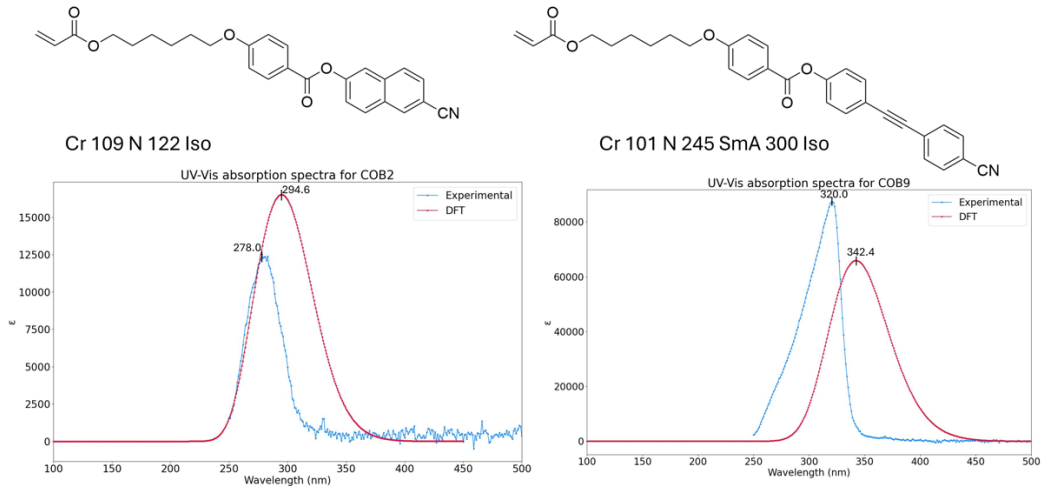

Figure 1: Comparison of transition temperatures and UV-Vis spectra for a liquid crystal with a naphthyl group (left) compared to a tolane group (right). Experimental UV-Vis spectra measured in 10 Î_M solution with methanol as the solvent. Calculated UV-Vis spectra calculated with DFT B3LYP/cc-pVDZ.

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Improving Supersaturation Control in Low-Solubility Systems: Integrating Machine Learning with Model Predictive Control

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Precise supersaturation control at fixed or dynamic setpoints is crucial for obtaining desired crystal properties in batch cooling crystallisation. A predetermined or real-time optimised supersaturation trajectory must be closely followed to achieve desired properties including crystal size. In low-solubility solute-solvent systems, chemometric techniques can suffer from reduced accuracy due to weak signal responses and measurement noise. This work investigates the integration of machine learning model-based predictive control (ML-MPC) with a weighted chemometric approach proposed to improve supersaturation regulation in these low-solubility systems.

An automated crystallisation rig was built for batch cooling crystallisation, incorporating a thermostatic bath for temperature control, PTFE Pt-100 temperature probe, FBRM, and ATR UV-VIS (see Figure 1). Python software controlled all system components, predictive models, chemometric analysis, and equipment commands. Experiments were conducted on a paracetamol in water batch cooling crystallisation, in an agitated 5-liter jacketed reactor. A comparison was undertaken between an Artificial Neural Network (ANN), Partial Least Squares (PLS), and a single wavelength derivative-based chemometric approach. A weighted method, combining each chemometric technique, was developed to improve chemometric robustness. Two temperature control methods of Proportional-Integral-Derivative (PID) control and MPC were compared for their efficiency in achieving and maintaining supersaturation setpoints, both static and changing. The temperature MPC was trained using a combination of mechanistically generated and empirical data.

The weighted chemometric method was found to be more accurate over the required conditions, via comparison with gravimetric analysis. Temperature MPC control was found to achieve improved supersaturation control over PID for each supersaturation trajectory, as shown in Figure 2. The temperature MPC improvement was found to be more pronounced for rapidly changing supersaturation setpoints, compared to static or gradually changing. Supersaturation MPC is proposed to be necessary to improve control, as temperature MPC, though accurate in its predictions in how temperature will change, cannot account for how supersaturation will change over the prediction horizon. The supersaturation rate of change must therefore likely also be considered in a predictive model.

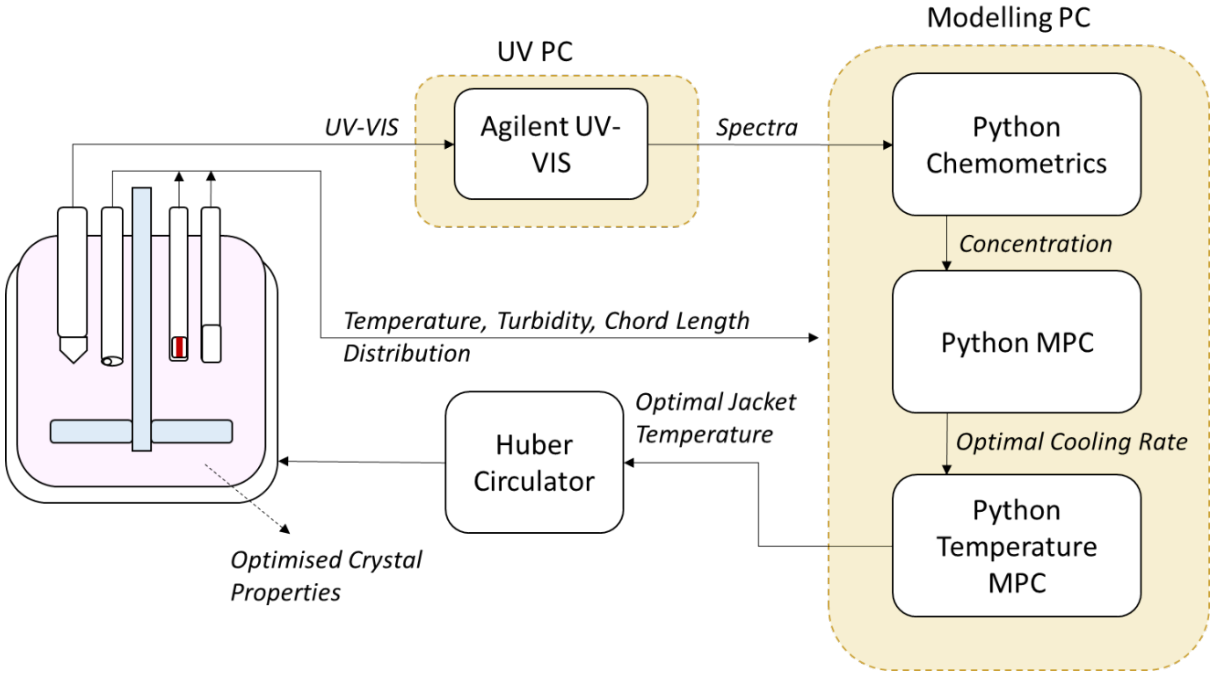

Figure 1 Flowchart of control method for supersaturation MPC

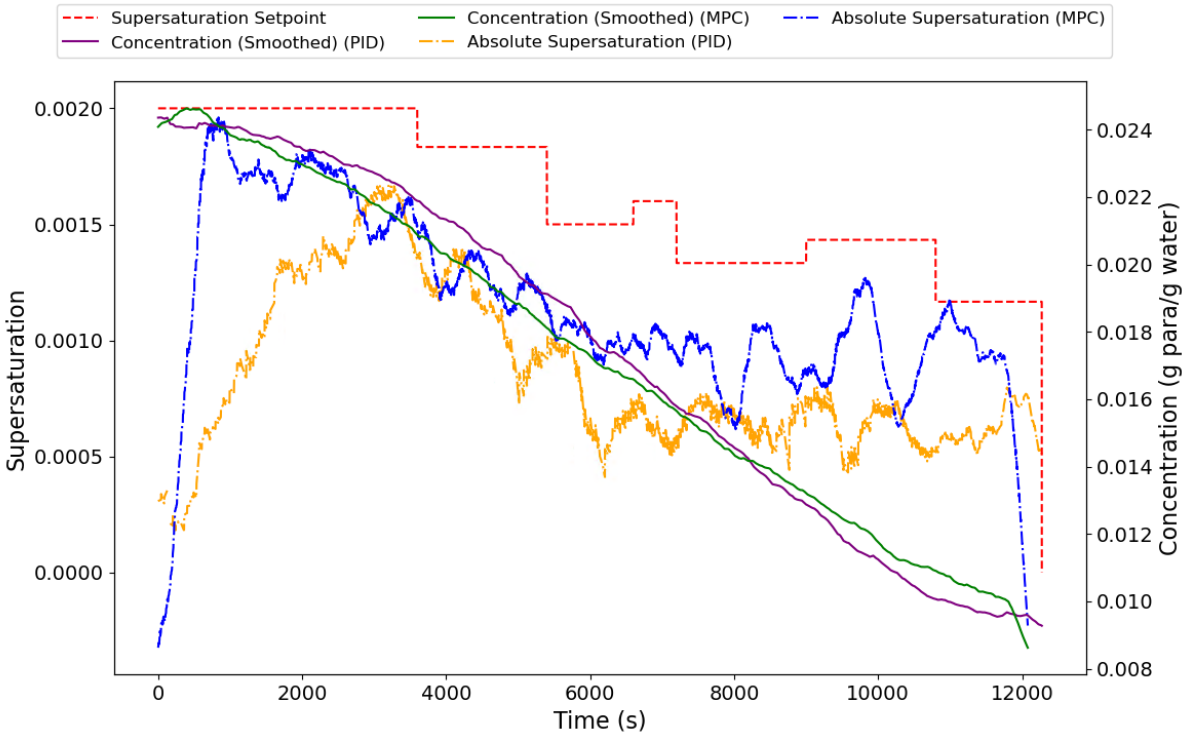

Figure 2 Absolute supersaturation profiles of PID compared to MPC temperature control of a paracetamol in water cooling crystallisation, during a gradual supersaturation setpoint change

Enhancing a Novel Carbon Capture Technology Using Open-Source CFD Modelling

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There is an urgent requirement for global decarbonisation efforts to be developed, improved and deployed as rapidly as possible to avoid irreversible environmental damage. Direct air capture (DAC) is an effective, scalable, and in this case, permanent method of carbon capture that can be utilised to remove significant amounts of carbon dioxide from the atmosphere. In this talk I describe the improvement of a DAC technology developed by Origen Carbon Solutions which utilises the processing of lime to capture and store CO2, using open-source CFD software OpenFOAM [1] to model the calcination of the calcium carbonate material within the system.

Multiple turbulence models are tested, evaluated, and implemented into a suitable Lagrangian particle model along with appropriate heat and mass transfer, chemistry, and combustion models to simulate the process as a whole. This will provide results on the efficiency of the system to allow refinement of specific variables. We also plan to implement machine learning techniques to support the processing of experimental data for the development of CFD-ML hybrid models.

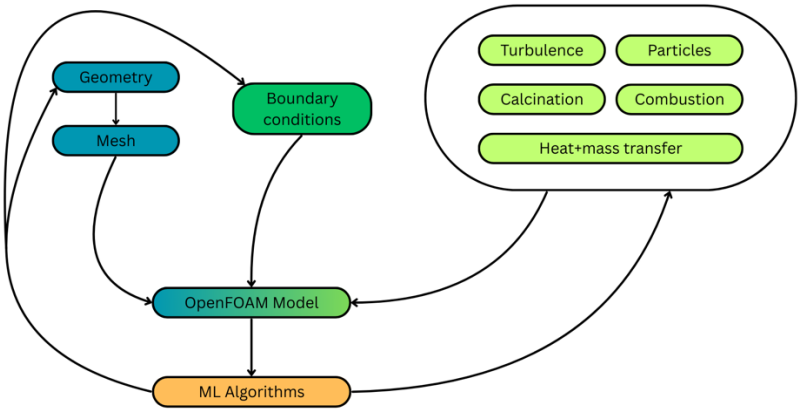

Figure 1: A diagram depicting a high-level view of the overall work flow for the project.

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Impact of plant-based wax crystal structure and morphology on physical property and stability of oleogels

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There is an increasing interest in incorporating biocompatible particles to stabilise water-in-oil emulsions to meet expectations of clean and green products. Plant-based waxes are attractive alternatives to synthetic emulsifiers offering functionality through Pickering or network stabilisation mechanisms via oleogelation of the continuous phase. Rice bran wax, RBX (melting temperature 76 °C) and rapeseed wax, RSX (melting temperature 56 °C) were used to prepare oleogels in sunflower oil (SFO). RBX has a 2D rectangular molecular packing structure with needle-shaped crystal morphology, while RSX displays a tighter 2D oblique molecular packing structure with a spherulite morphology on microscale. A minimum of 10 wt% RSX is needed to form self-standing oleogels in SFO using the crystallisation rig which is nearly double the concentration of RBX. The interfacial tension between the SFO and water decreases by nearly 5 mN/m upon the addition of waxes. Ongoing studies investigate the impact of wax morphologies within the oleogels on their organisation at water-oil interface by microscopic visualisation of in situ crystal formation at the surface of a single water droplet.

Acknowledgements: Authors gratefully acknowledge the Engineering and Physics Sciences Research Council (EPSRC) funded Centre for Doctoral Training in Molecules to Product, Grant Ref. No. EP/S022473/1 for financial support.

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6th Annual Inter CDT Conference 2025
26 – 27th June 2025
University of Cambridge

Bacterial Motility and Membrane Deformation in Biohybrid Vesicles

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We investigate bacterial interaction with lipid membranes in the context of intracellular bacteria invading host cells. Using biohybrid vesicles encapsulating E. coli within artificial lipid vesicles, we model bacterial-driven membrane deformations and self-propulsion [1]. Bacterial motion generates forces that deform the membrane, with the extent of deformation dependent on bacterial density and motility [2]. We aim to explore vesicle motion in chemical gradients, driven by chemotactic bacteria, which results in asymmetric bacterial distributions and vesicle propulsion. A flow-free microfluidic system establishes pH gradients [3], allowing bacteria to exhibit chemotaxis within the vesicle lumen [4]. We propose two mechanisms for vesicle motion: (i) flagellar bundling creating helical propellers that couple with the membrane, or (ii) asymmetric bacterial accumulation generating a collective force for directed movement. These behaviours are influenced by bacterial swim pressure and vesicle membrane tension. This study advances understanding of bacterial interactions with lipid membranes and informs smart drug delivery system design.

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From Tip to Ship: Characterisation of New Marine Antifouling Coatings After Aging

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Biofouling is a well documented problem on marine structures, with fouling of these surfaces increasing costs as well as reducing the operational lifetime of structures. Common antifouling strategies rely on biocides, killing fouling organisms coming in close contact with the coated surfaces during the early stages of biofouling, however these are known to have detrimental impacts on marine ecology. One alternative entails physical methods, where the coating's varying surface energies prevent binding of fouling organisms to the surface. However, many new strategies cannot easily be scaled up for routine use in industry. Herein, we investigate a promising new strategy for a polymer-based antifouling coating that combines particular mechanical properties together with nanoscale control of the surface amphilicity. This strategy can easily be scaled up, however its specific mode of action and evolution after aging are not fully understood. Using Atomic Force Microscopy in solution, we characterise differences between candidate coatings, quantifying nanoscale structural and viscoelastic properties after aging in seawater to reveal changes in these coatingsâ€™ characteristics over time.

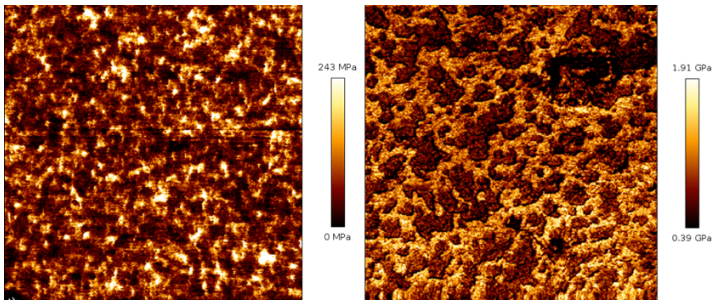

Figure 1: Two atomic force microscopy (AFM) images showing aging of a prototype antifouling coating over 1 week. The left image is an unaged sample and the right image is a sample aged over 1 week. These images show the estimated Young's Modulus according to the colour scale.

Acknowledgements: This project is partly funded by AkzoNobel Coatings Limited.

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Evolutionary Optimisation of a Pharmaceutical Feeder System

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This project focuses on the feeding stage of continuous direct compression, a challenge due to the absence of intermediate operations to improve the flowability of the matter.

The aim is to develop a well-validated in-silico DEM model of a twin-screw loss in weight feeder using a simple, free-flowing powder. Positron emission particle tracking (PEPT) will be used to image a radioactive tracer within the system to gain an insight into its internal dynamics. Various powder characterisation tools, along with their digital twins, will be used to calibrate the measurable powder properties with the corresponding in-silico parameters. The most suitable characterisation tool for this system can then be established by comparing the model with the post-processed PEPT data and determining which characterisation tool leads to the most accurate calibration.

Once a suitable characterisation method has been established, powders with more complex flow behaviours can be placed into the model. The use of an evolutionary algorithm can then be used to optimise the geometries of equipment, with the purpose of minimising the influence of material attributes on the overall process robustness.

Optimising PAT for Continuous Direct Compression using a Feed Frame Simulator

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Monitoring formulation quality during Continuous Direct Compression (CDC) to maintain product specifications is complex. Critical Quality Attributes (CQAs) are controlled by adjusting Critical Process Parameters (CPPs). Determining appropriate CPPs can be improved by an enhanced control strategy using chemometric modelling and Process Analytical technology (PAT), allowing in-line CQA monitoring and reducing time for off-line analysis.

This work optimises PAT for CDC, integrating spectroscopic techniques into the feed frame simulator. By employing Near-Infrared (NIR) spectroscopy, Raman spectroscopy and NIR-Spatially Resolved Spectroscopy, the accuracy and efficiency of the technologies and resulting models are enhanced, ensuring consistent product quality.

Key steps include optimising acquisition parameters such as integration time across technologies, enabling model development with Partial Least Squares regression. A sensitivity comparison of these technologies based on optimised parameters for given drug formulations is critical. By standardising data analysis methods and developing a real time release testing strategy, the project addresses current PAT application challenges.

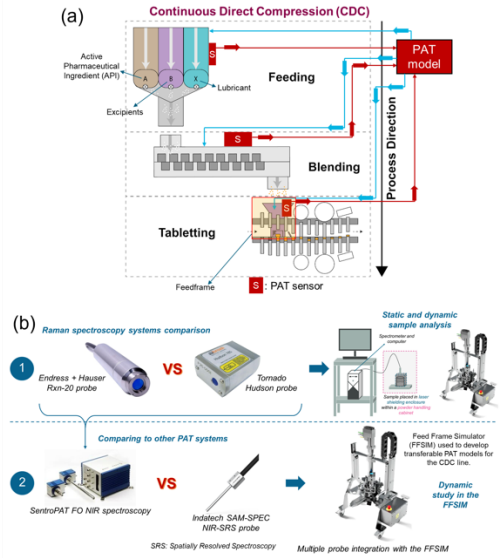

Figure 1: (a) Project aim of developing an integrated Real Time Release Testing PAT strategy for the CDC process and (b) Current work package on Raman and Near Infrared Spectroscopy technology comparisons.

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Reengineering PLFs: Molecular Upcycling

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Polymers in Liquid Formulations (PLFs) underpin countless everyday products—from paints and inks to detergents and adhesives—yet remain largely unknown to the public. Despite their prevalence, PLFs are environmentally unsustainable, with ~36 million tonnes produced annually from fossil feedstocks. Used in a linear economy, $125 billion USD worth of PLFs never recovered each year.

This work focuses on the chemical recycling of RAFT (Reversible Addition–Fragmentation chain Transfer) polymers. While RAFT is a powerful and widely used controlled radical polymerisation method, its sustainability depends on regenerating monomers from end-of-life materials. We are developing efficient depolymerisation strategies in continuous-flow to demonstrate the recyclability of RAFT polymers and support a circular economy.

To add further value, enzymatic biocatalysis is being explored to upcycle recovered monomers into higher-value compounds. The goal is to integrate depolymerisation and biotransformation into a fully continuous process, using online analysis for real-time monitoring and optimisation. This approach aims to reduce waste and generate value-added products from end-of-life PLFs.

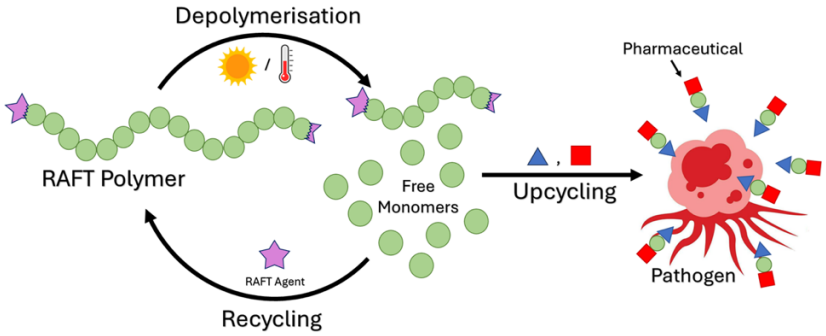

Figure 1: Pathways of recycling and upcycling RAFT polymers

Acknowledgements: EPSRC and Molecules to Product CDT (Grant Ref. No. EP/S022473/1), the Clayton Group, the Warren Group, other members of the iPRD

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Strip Casting of SmCo Alloys to Reduce Manufacture Costs of $Sm_2(Co,Fe,Zr,Cu)_{17}$ Permanent Magnets

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Samarium Cobalt (SmCo) magnets currently are conventionally book mould cast, causing the formation of an inhomogeneous crystal structure. The cast alloy must be mechanically crushed and milled to yield powder for sintering. Following the sintering to a fully dense body, a solution heat treatment is required to produce a $SmCo_5$ hexagonal (1:5H) and $SmCo_7$ hexagonal microstructure. This is then quenched and aged where the microstructure precipitates out the nanostructure of a sintered Sm_2Co_{17} rhomboidal magnet.
The microstructure produced from the strip casting of SmCo alloys has shown a similar phase composition to that of solution heat treated Sm_2Co_{17} which could make this step of manufacture redundant, reducing production costs. In addition, the 1:5H phase has been seen to be the most susceptible to hydrogen decrepitation making it less energy intensive to produce sintering powder.
In this project the texture of the strip cast wheel was analysed and was seen to affect the nucleation behaviour in the flake leading to changes to the microstructure. Influencing the nucleation behaviour of dendrites is key to forming an optimal cast microstructure.

Development of sustainable hair conditioning technologies

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This study explores silicone oil (Si-Oil) in hair conditioning, examining its spreading and wetting kinetics to help develop bio-derived alternatives. Using the Wilhelmy plate method and contact angle goniometry, it analyzes the surface tension of 10 silicone oils, aiming to identify effective bio-derived models.
Different models have been explored to describe the maximum spreading parameter $\beta_{max} = D_{max}/D_0$ as0 as a function of non-dimensional numbers, such as the Reynolds number (Re)=($\rho V D_0)/\eta$ and the Weber number (We) = $\rho V^2 D_0/\sigma$. Most models in the literature are restricted for Re >100 , and most. Most of the experimental data in the set of selected silicone oils lay Re<below 10. After correlating and fitting the experimental data with power law, it was observed that βmax scaled with $Re^{0.05}$ and $We^{-0.3}$. It was observed that we played a more dominant role in determining spreading effectiveness compared to Re, which could be attributed to a similar rheology. This emphasised the critical role of surface tension-driven forces in the spreading dynamics of the silicone oils.

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Nanomechanical measurements of solid fabric enhancer (SFE)

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Solid Fabric Enhancers(SFE) are applied onto garment surfaces during the tumble drying process to reduce static build-up on fabrics and lubricate fibres. In this study, SFE coatings (15μm thick), composed of quaternary ammonium ester(EQ) and fatty acid(FA), were prepared on PET substrates. Their nanomechanical properties were assessed using atomic force microscopy (AFM)-based force spectroscopy, essential for evaluating the delivery efficiency of SFEs. Two types(A and B) of both EQ and FA were used, each exhibiting distinct mechanical characteristics. While both FAs had similar adhesion (5.0nN vs 5.1nN), their Young's modulus differed significantly(3.3MPa vs 6.1MPa). For EQs, Young's moduli were similar(1.8MPa vs 1.6MPa), but adhesion varied (6.5nN vs 12.6nN). Consequently, the A and B mixtures displayed different behaviours. Nanoindentation data revealed that the AFM tip penetrated layers with varying stiffness, indicating that molecules organize near the surface. These measurements show individual components adopt distinct molecular configurations, influencing the structural features and performance of soft solid formulations used further in consumer goods and healthcare sectors.

Acknowledgements: Authors acknowledge financial support received from the Centre for Doctoral Training in Formulation Engineering (EPSRC grant no. EP/S023070/1).

Enhancing the Penetration of Cosmetic Actives into the Skin

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Many commercial cosmetic skincare products contain active ingredients to treat and/or prevent certain non-clinical skin concerns. However, effective penetration of the active ingredient into the skin is not readily achieved due to the protective outer layer of the skin. The project aim is to develop skincare formulations with improved skin penetration of the active ingredient to achieve effective delivery to the target area. Currently, efforts to overcome this issue of limited penetration include increasing the quantity of active in the formulations which is not sustainable. Hence, it is important to understand how active ingredients can be delivered more effectively to the skin. Different formulation methods to enhance skin penetration of actives will be explored, such as, incorporating penetration enhancers and using different delivery systems. Textural attributes and mechanical properties of the formulations will be assessed using tribology and rheology. Skin models, from basic skin mimics, advancing towards 3D printed skin layer substitutes, will be developed to assess the quantity of active and depth of delivery to provide an alternative to current human-testing methods.

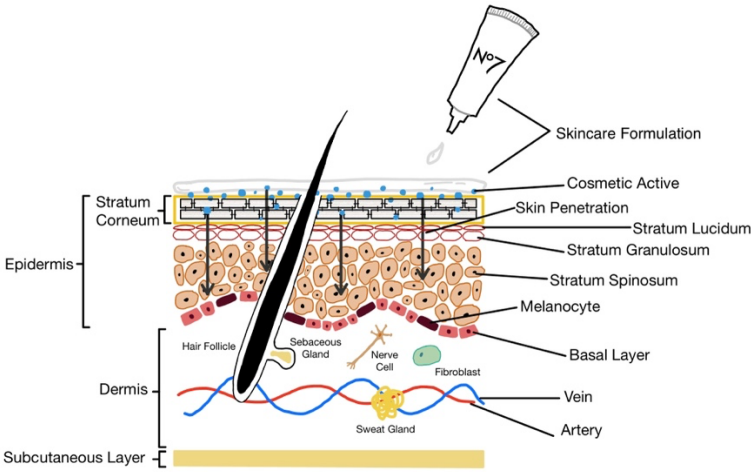

Figure 1: Illustration of skin penetration of actives from a cosmetic formulation as intended to be achieved within this project - adapted from Tambunlertchai S et al.

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Characterisation of iron oxides in red gypsum using TEM: Towards valorisation of TiO_2 co-products

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Red gypsum as a co-product of titanium dioxide manufacture is an alternative to mined gypsum for applications in agriculture, construction and land remediation[1,2]. Neutralisation of spent sulfuric acid rich in dissolved iron produces micrometre sized gypsum crystals and a nanoscale fraction of primarily precipitated iron oxides[3]. Due to a lack of spatial specificity and the dominance of crystalline gypsum, bulk diffraction techniques struggle to identify nanocrystalline iron (oxyhydr)oxides. Understanding of the fine phase is essential in valorising red gypsum as it can contribute to poor filtration and undesirable rheology. In this work this industrial red gypsum was characterised to determine elemental composition and phase morphology, as well as rheological behaviour of suspensions. Selected Area Electron Diffraction can resolve the nature of the fine fraction. Two phases were identified: a needle-like lepidocrocite with low impurity levels, and an agglomerated, poorly crystalline ferrihydrite with high levels of associated titanium. These insights will be used to produce model systems of red gypsum where phase morphology is controlled and its influence on rheology determined.

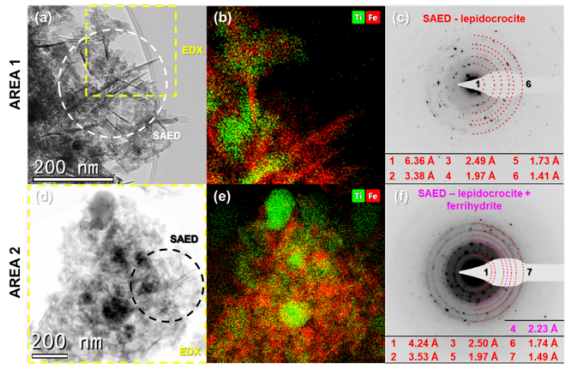

Figure 1: Transmission Electron Microscopy (TEM) of red gypsum fines: (a) image of Area 1 with needle-like and agglomerated iron oxide phases, (b) Energy Dispersive X-Ray (EDX) map from highlighted section in Area 1 of titanium and iron distributions showing an iron rich phase and an iron/titanium mixed phase, (c) Selected Area Electron Diffraction of the needle-like phase indexes to lepidocrocite, (d) image of area 2, (e) titanium and iron EDX map of area 2 showing titanium dioxide particles and mixed phase, and (f) SAED pattern from Area 2 indexes to lepidocrocite and ferrihydrite.

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Understanding the Barocaloric Effect in Polymers with Molecular Dynamics

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Current refrigeration processes consume over 20% of the global energy usage and emit high global warming potential gases. [1] This is unsustainable, so new refrigerants must be developed to avoid further global warming emissions and meet the growing demand. [2] Solid state refrigerants are a long-term solution, with the most promising being materials with a “massive” pressure-induced caloric effect: barocaloric effect (BCE). [3] The BCE is observed in polymers, and this work focuses on nitrile butadiene rubber (NBR). [4] Using polymers as refrigerants is an exciting avenue towards recycling and reusing otherwise-polluting refuse. [5] There is little experimental, and less computational, work on barocaloric polymers so the exact origins of their “giant” BCEs are unknown. [6] The BCE in polymers, specifically adiabatic temperature change (ΔT_{ad}), is affected by the glass transition temperature (T_g), above and below which we consider the polymer a rubber or glass respectively. We explore how copolymer ratio affects the BCE in NBR melts across their glass transition temperature domains using molecular dynamics simulations.

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Exploring Discharge Product Distribution in Li-O_2 Batteries

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Li-O2 batteries are a post-Li-ion battery technology which promise extremely high energy densities (>3000 Wh/kg) [1]. Many technological problems must be overcome before they are commercially viable, one of which is limited capacity at high discharge rates due to slow mass transport of O2 through the air electrode, resulting in low overall utilisation of the air electrode. We have used scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) and X-ray micro-computed tomography (microCT) to characterise the discharge product distribution throughout the air electrode, exploring different discharge rates and electrolyte solvents. The findings suggests the distribution is dependent on a combination of O2 mass transport and Li2O2 nucleation and growth kinetics. We have developed a continuum model of the Li-air battery air electrode which more accurately captures the Li2O2 morphology, and the distribution of Li2O2 in this simulated electrode matches more closely with our experimentally observed results, when compared to existing models [2]. These results will allow for improved rational design of electrolytes and electrode structures.

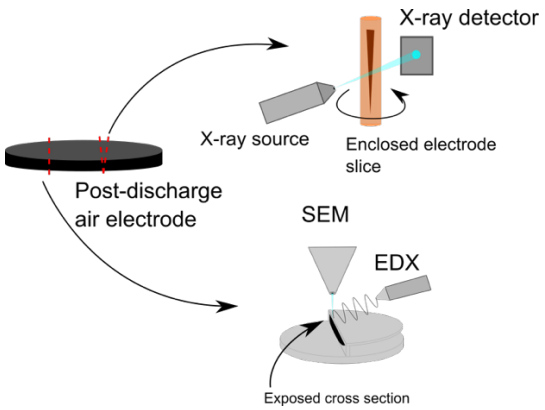

Figure 1: Experimental setup for characterisation of discharge product distribution using X-ray microCT and SEM-EDX

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Using iPSC-derived Motor Neuron as a model to investigate the pathological effect of mutant Fused in Sarcoma (FUS) on the cellular calcium and organelle dynamics in Amyotrophic Lateral Sclerosis (ALS)

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Amyotrophic Lateral Sclerosis (ALS) is a fatal disease characterised by the selective degeneration of motor neurons in the brain and the spinal cord. Mutation in the Fused in Sarcoma (FUS) protein is commonly associated with juvenile onset ALS, and the pathology is not yet well understood. Of which the R495X mutation is especially clinically aggressive and associated with rapid disease progression. We model this type of FUS-ALS by differentiation pluripotent stem cells with R495X point mutation into human spinal motor neurons. Using calcium and organelle specific dyes we can visualise cellular calcium dynamics and organelles such as mitochondria to examine the pathology of FUS-ALS on human neurons.

Liquid Foams in Motion: Probing Multiscale Rearrangements with Adhesion Tensiometry

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Understanding the dynamics of liquid foams across scales is essential for connecting macroscopic rheological behaviour with underlying microscopic structural rearrangements. In this study, we investigate foam (10% sodium dodecyl sulphate foam [1]; liquid volume fraction ~10-20%) evolution using a vertical adhesion tensiometry setup, where a foam bridge forms and evolves between a moving plate and a static holder. By combining high-resolution force measurements with frame-by-frame image analysis, we track intensity changes as proxies for bubble rearrangements and rupture events. We were able to directly correlate individual force drops with image-derived events, suggesting force drops are linked to observable microstructural events. Preliminary statistical analysis reveals that the distribution of force drops exhibits signatures of scale-invariant behaviour, including lognormal and power-law regimes. We believe this suggests a transition region between exponential (bubbly liquid) regime and power-law (dry foam) regime. These findings motivate a deeper understanding of foam dynamics, which is essential for the design and development of more stable and sustainable foam-based products.

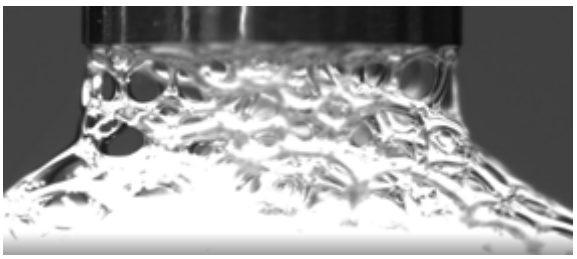

Figure 1: Adhesion tensiometry set-up between foam bubbles to capture the bubble-scale dynamics.

Acknowledgements: I would like to thank SOFI2 CDT and EPSRC for the funding and support.

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Enzymatic degradation of proteinaceous Pickering particles – a strategy to induce demulsification

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Although Pickering emulsions stabilized by food-grade particles have gained interests due to their ultrastability; the process of demulsification, critical for releasing active ingredients from those droplets, has received limited attention. This study aimed to understand demulsification of Pickering emulsions using a particle dissolution approach by enzymatic degradation [1]. We hypothesized that trypsin, will reduce the size of whey protein microgel particles (WPM), reducing desorption energy and inducing droplet coalescence. The capability of trypsin to digest WPM was monitored at pH 7.0 varying conditions (enzyme ratio, concentration, treatment duration) using DLS, drop tensiometry, SDS-PAGE, atomic force microscopy (AFM), confocal laser scanning microscopy (CLSM) and interfacial shear rheological analyses. Results showed that exposure to trypsin led to a decrease in WPM size by 41%, a similar trend was observed in reducing interfacial shear viscosity. Interfacial film thinning of the degraded microgel resulted in droplet coalescence, showing promise of enzymatic degradation as a demulsification strategy unlocking new possibilities in release of actives such as nutraceuticals.

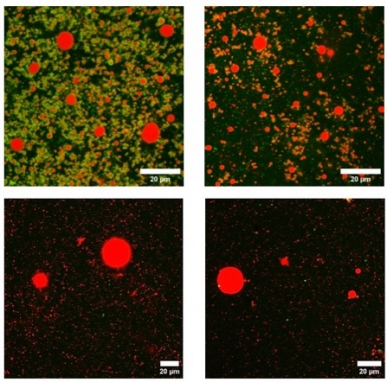

Figure 1: Confocal images of emulsions stabilised by WPM (a), digested by Trp (1.25 mg/ ml) (b), Trp (3.75 mg/ mL) (c) and Trp (5 mg/ ml) (d). Red droplets are dyed by Nile red, Fast green and in all samples are taken after 2 h digestion.

Acknowledgements: Authors gratefully acknowledge the Engineering and Physical Sciences Research Council (EPSRC) funded Centre for Doctoral Training in Molecules to Product, Grant Ref. No. EP/S022473/1 for financial support.

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Synthesis and analysis of transition metal pyrithiones and pyridineselenones to address antimicrobial resistance

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Studies have used copper salts and complexes as adjuvants to address the growing threat of antimicrobial resistance.[1]
Ionophores such as copper pyrithione have recently been demonstrated to act as potent antibacterial agents;[2] they inhibit β-lactamase enzymes (such as New Delhi metallo–β-lactamase (NDM1)) through mis-metalation of the zinc in the enzyme's active site. However, key issues remain with regards to aqueous solubility, bacterial uptake and selectivity, and toxicity of these metallodrugs limiting their applicability in medicine. This project aims to introduce small functional group modifications of the pyrithione ligands to increase lipophilicity and thus bacterial uptake, as well as increase the bound metals from copper to other 2+ transition metals (Mn, Ni, Zn, Cd). The metal binding sulphur atoms in these ligands have also been replaced with selenium to create novel selenone complexes to further increase stability and selectivity.
Furthermore, drug loaded micelles have been formulated to address solubility issues. PEG-PCL Diblock copolymers have been synthesised by ring opening polymerisation and self-assembled around the active metal complexes.

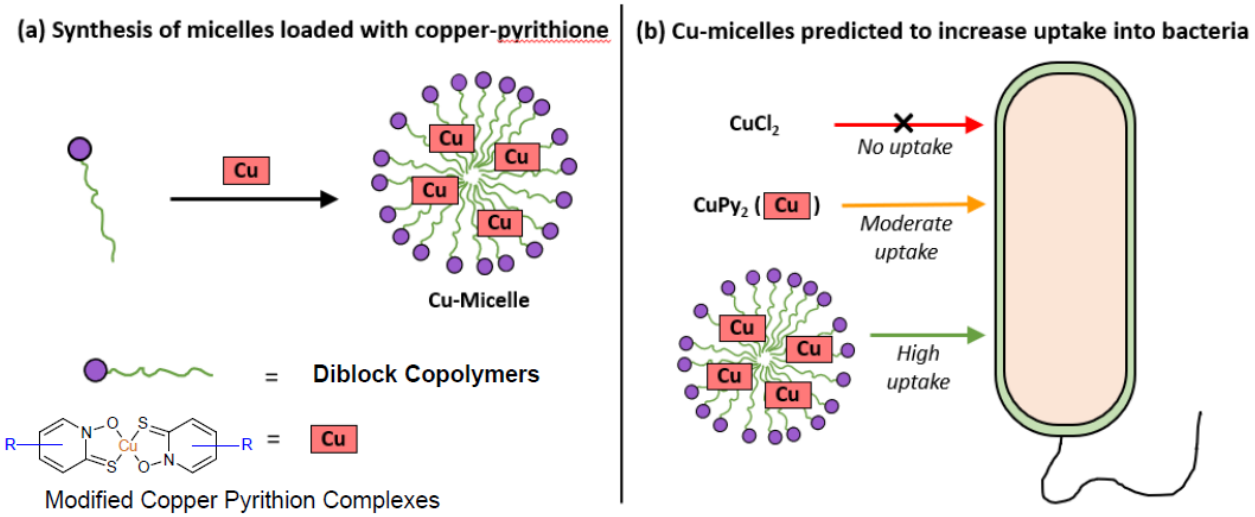

Figure 1: (Left) Figure showing the encapsulation of modified copper pyrithiones into polymeric micelles. (Right) Increased uptake and bactericidal activity from encapsulated complexes in comparison to copper salts.

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Tough meets Stretchy: towards systematic control of threaded γ-CD for slide-ring materials

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Gamma-cyclodextrins (γ-CDs) promise synthesis of slide-ring gels (SRGs)- polymeric networks linked by supramolecular 'pulley' crosslinks, constructed of rings threaded by the network's strands- in fewer steps. Unlike conventional 'figure of eight' singly threaded systems, γ-CD enables a concerted threading and crosslinking process by the double-threaded topology of the large cavity by poly(ethylene glycol).[1-2] However, despite their potential to enhance mechanical properties, γ-CDs remain underutilised due to challenges in reliably controlling the double-threading process.[3-4]
This work employs rheology to investigate key interactions governing γ-CD threading and their impact on material properties. Using minimal-component model polypseudorotaxanes, we establish a structure-function relationship between γ-CD threading and mechanical behaviour. Our findings demonstrate the critical role of chain-end-to-ring interactions in conjunction with double-threading for effective gel formation. These insights provide a pathway for designing tougher and more extensible SRGs with tuneable properties, further enhancing the impressive mechanical properties previously displayed by SRGs.[2][5]

Acknowledgements: Special thanks to Professor Chenfeng Ke (now of Washington University in St Louis), and to SOFI2CDT, UK Research and Innovation (UKRI), and Reckitt.

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Bayesian Optimization for Automatic Tuning of Sensor Dots in Silicon Quantum Dot Arrays

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Silicon spin qubits are a promising platform for scalable quantum computing, primarily due to the advantages of CMOS-compatible fabrication and established semiconductor technology. A critical component in these quantum dot array systems is the use of sensor dots, which enable high-fidelity readout of charge states by detecting electron transitions through variations in gate voltages. However, tuning sensor dots remains a challenging and time-consuming task, typically requiring manual adjustment of multiple gate voltages in a high-dimensional parameter space.

In this work, we present a fully automated method for tuning sensor dots using Bayesian Optimisation (BO), which explores the gate voltage landscape to identify optimal sensing peaks with minimal experimental overhead. We demonstrate the success of this approach across over 40 devices, achieving reliable tuning based on a single gate voltage. Furthermore, we extend our method to higher-dimensional tuning problems, including a demonstration involving five gate voltages. Our results highlight substantial time savings and improved scalability, paving the way toward fully automated calibration of large-scale quantum dot arrays.

Forging Fusion-Grade Steels in the 3D Printer: The Power of In-Situ Control

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Additive manufacturing (AM) opens up new possibilities for producing complex, high-performance steel components, yet controlling the microstructure required for extreme environments such as fusion reactors remains a significant challenge. This work focuses on forging fusion-grade steels directly during 3D printing via in-situ microstructure control. We explore strategies for tailoring material properties—including phase control, precipitation strengthening, and defect density—by dynamically adjusting thermal profiles and laser processing parameters. By tuning key variables such as heat input and cooling rates we demonstrate the ability to trigger critical phase transformations and microstructural refinement directly during fabrication. This work establishes a new paradigm for adaptive, performance-driven additive manufacturing of steels, bridging the gap between process control and the material performance demands of next-generation fusion energy systems.

Lights, Camera, Droplets! Platform development to study impact behaviour on a pleural tissue phantom

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Respiratory diseases are among the leading causes of death worldwide 1. For treatment, the delivery of aerosolized drugs has shown promise, but further studies on drug screening and efficacy are required. To this end, in vitro biological models, varying in physiological relevance and throughput, have been developed to mimic the in vivo system of interest and the ways treatments interact with them.
Here, we study clinical procedures required for aerosol delivery of chemotherapy drugs and identify key areas where research is needed to bridge the gap between concept and translation. In particular, we focus on developing lab-based measurement devices to understand (i) aerosol delivery to respiratory spaces, and (ii) aerosol-tumour interactions.
A hydrogel is formulated to mimic the membrane lining the lungs. The interactions of droplets with this hydrogel are imaged using a custom-built high frame rate and high magnification imaging setup. These initial results and the experimental tools developed are the first steps towards creating more complex hydrogel-based in vitro models to accelerate translation at the intersection of personalized medicine and targeted drug delivery.

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Formulation engineering of enhanced sustainability beverage emulsions

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Beverage emulsions are broadly classified into two major types: clear (low turbidity) flavour emulsions and cloudy emulsions. This research focuses on the formulation of low-turbidity emulsions specifically designed for flavour delivery in beverages. Achieving optical clarity requires the effective encapsulation of hydrophobic flavour molecules, where a minimum droplet size is necessary to maintain its stability in the aqueous phase. The key challenge lies in developing emulsification methods of producing low-turbidity flavour emulsions that effectively deliver flavour compounds. Emulsions with droplet sizes below 100 nm are promising due to their ability to maintain optical clarity while dispersing hydrophobic flavour compounds in aqueous systems. However, achieving optical clarity represents only a partial solution; it is equally essential to optimise the formulation of surfactants and co-surfactants in conjunction with hydrophobic flavour compounds, fine-tuning their optimal ratios and processing parameters to facilitate controlled flavour release within the beverage matrix.

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Deformation relaxation dynamics in dioxaborolane vitrimers

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Vitrimers have attracted widespread interest over the last decade due to their intriguing properties and promising role in facilitating a circular material economy [1]. However, the mechanisms by which vitrimers reorganise their macromolecular structure are often not fully understood.

Recent literature has reported vitrimers that show excellent material properties which can sometimes be attributed to the dynamic crosslink exchange, though how these properties arise is not well understood [2,3]. A deeper understanding of how these materials adjust to respond to external deformation would provide more insight into how these materials perform over longer durations and their fracture behaviour [4].

Here, we present the synthesis and characterisation of a class of vitrimers which exploit dioxaborolane metathesis to achieve dynamic bond exchange. Tensile and rheological tests were performed to determine their linear response, as well as their behaviour under deformation. We also explore whether the application of both small and wide-angle X-ray scattering alongside birefringence studies can give insights into how the material structure varies under different degrees of deformation.

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PD-L1 Nanoparticle Protein Degrader for targeting Chemotherapy-Induced Senescence

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Senescence is a state of cell cycle arrest that arises as a damage-response to various insults, including chemotherapy, which is usually regulated by immunosurveillance. Persistent senescence occurs when routine immunosurveillance fails, which worsens cancer prognosis by assisting metastasis and contributing to chemotherapy resistance. [1] One of the means which senescent cells evade immunosurveillance is by PD-L1 upregulation, which suppresses killer T-cell cytotoxicity. [2] Although various PD-L1 inhibitors exist, they only work on some patients and may induce off-target adverse effects. [3] Using the concept of lysosomal targeting chimeras (LYTAC) [4], this project aims to use antibody-conjugated nanoparticles to direct PD-L1 on senescent cells to their lysosome, hence achieving targeted PD-L1 degradation (Figure 1). At present, the nanoparticles required were successfully synthesised and preliminary PD-L1 degradation has been shown on breast cancer cells. Successful development of this degrader will enable senolysis in chemotherapy-induced senescence with minimal off-target side effects, and potentiates broader applications in other senescence-related conditions such as ageing.

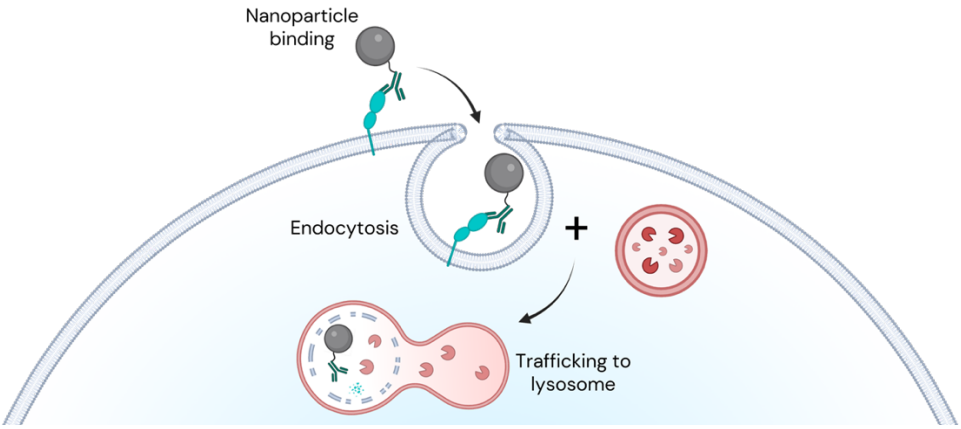

Figure 1: Insert Proposed mechanism of the nanoparticle protein degrader to degrade PD-L1 through the lysosomal pathway.

Acknowledgements: EPSRC. Grant Number: EP/W035049/1, EPSRC NanoDTC. Grant Number: EP/S022953/1

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Novel Characterisation of Topographically Complex Metal Additively Manufactured Implant Surfaces

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Metal additive manufacturing (AM) and its associated design freedoms have facilitated a rapid industrial uptake, especially in the context of architecturally complex and patient specific orthopaedic devices. Laser Powder-Bed Fusion (LPBF) is a metal AM sub-category, based on laser consolidation of metallic powder feedstock, used to produce osseointegrative lattices and tailored implant geometries. However, surface adhered particle defects, inherent to powder AM, hinder wider application; especially in medical device contexts, where surfaces greatly influence implant successes. Retained surface particles potentially pose risks in contributing to metallic debris release and osteolysis; hence, requiring accurate definition to inform postprocessing or manufacturing requirements. Conventional characterisation techniques suffer when applied to metal AM components due to hierarchal topographies, partially consolidated particles hide “true” underlying surfaces, and internal geometries are inaccessible by line-of-sight methods. Furthermore, top-down imaging cannot distinguish between embedded and partially attached particles, and therefore their respective potential detachment risk.

Herein, micro-computed tomography (MicroCT) was employed as a through thickness characterisation method to provide quantification of surface adhered particles. Local thickness analysis was applied to samples representative of implant geometries; circular shells at differed build angles and conformal lattices.[1] Consolidation laser line energy variation ([J.mm-1]; power [W] / speed [mm.s-1]), resulted in a 64% range in quantity of identified adhered bodies on simple geometries. With increasing build angle, 75 ° to 90 °, the measured surface particle quantity increased 135%.

MicroCT and subsequent analyses demonstrated the capacity to differentiate surface adhered particles from consolidated bulk structures on AM components. Furthermore, the contribution of build angle to particle adhesion, as well as the dependence on consolidation energy was observed, reinforcing the importance of parameter selection.

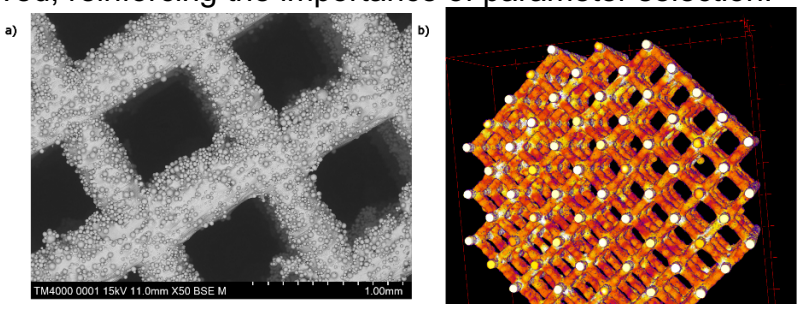

Figure 1: a) SEM micrograph of a Titanium-6Al-4V LPBF lattice, showing surface adhered particles, b) a subsection of the same lattice under microCT, subsequent to colourisation of residual surface particles using local thickness analysis [1]

Acknowledgements: The UK-EPSRC CDT in Topological Design and Renishaw

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A mesoscale approach to dynamic protein unfolding during gel network formation

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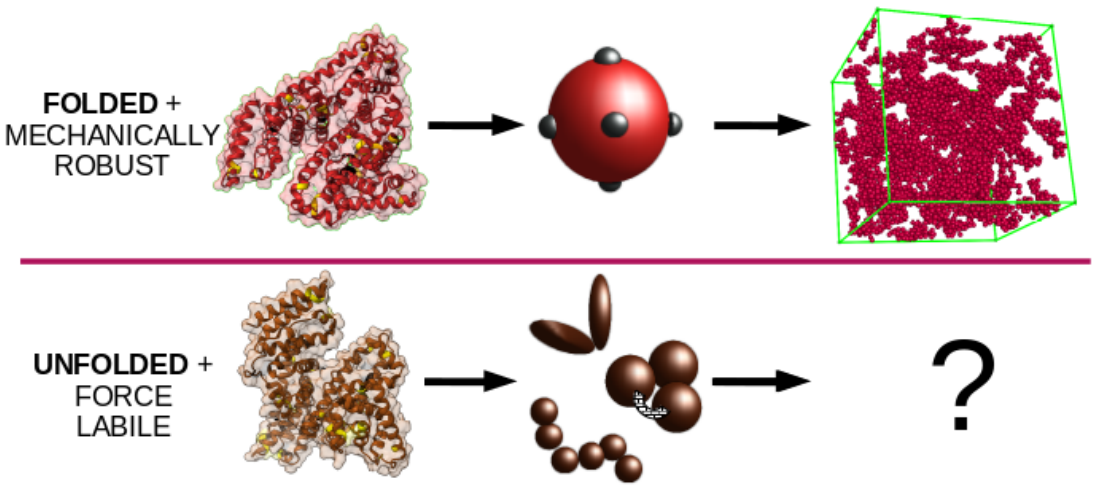
Globular protein hydrogels are highly versatile and can be rationally designed to suit specific applications such as tissue engineering, wound healing and body sensors. One of the ways in which we can control the mechanical properties of protein hydrogels is by controlling whether or not the proteins can unfold during gelation: gels with mechanically robust proteins that remain folded are stiffer and stronger; whilst gels with force-labile proteins that can unfold are more elastic [1]. However this is insufficient to be extensively able to control the mechanical properties of the gel – it is the process of proteins unfolding during network formation that can most strongly contribute to the gel's macroscopic properties [2], but this topological change is difficult to experimentally characterise. As such, we first introduce correlations between the mesoscale and macroscale gel network and discuss the significance of the mesoscale, as well as some challenges for modelling dynamic conformational changes. We then suggest a coarse-grained mesoscale model to represent a conformational change during gelation. By refining this *in-silico* method the contributions of protein unfolding during network formation will be more accurately quantified and controlled.



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[2] Hughes et al. JCIS 2025, 678 C, 1259-1269

Probing the electrical characteristics of passivated InAs nanowires using terahertz time-domain spectroscopy

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InAs nanowires' (NWs) high charge carrier mobility, narrow bandgap and relative ease of forming Ohmic contacts makes them an attractive material for electronics and optoelectronics [1]. While the NW geometry enables much of InAs NWs' appeal, their high surface-to-volume ratio also results in a large amount of surface defects which limits their potential.

This large density of surface defects results in strong charge accumulation on the surface, also termed Fermi level pinning as the Fermi level at the surface of the NWs is fixed within the conduction band [2]. This leads to unintentional n-type behaviour, reduced carrier lifetimes and mobility, and increased leakage currents. Furthermore, this accumulation layer reduces the ability to modulate the NWs as field-effect transistors due to electric field screening and difficulty in controlling its threshold voltage.

Alumina passivation via atomic layer deposition (ALD) has been shown to be a simple and effective way to eliminate this Fermi level pinning, restoring intrinsic positive photoconductivity to the InAs NWs [3]. However, the electronic properties of passivated InAs NWs have not been explored, such as their carrier density, mobility and lifetime, and carrier diffusion length. In addition, how the parameters of the passivation layer, such as passivation thickness and type of passivation layer affects these properties has not been explored. This presentation will explore the effectiveness of Al_2O_3 and MoO_3 passivation, and the dependence of nanowire electronic transport on the passivation layer's deposition parameters. We employ optical pump terahertz probe (OPTP) to extract carrier dynamics information with picosecond temporal resolution in a contact-free fashion. Al_2O_3 and MoO_3 passivation are also demonstrated to modulation-dope the nanowires.

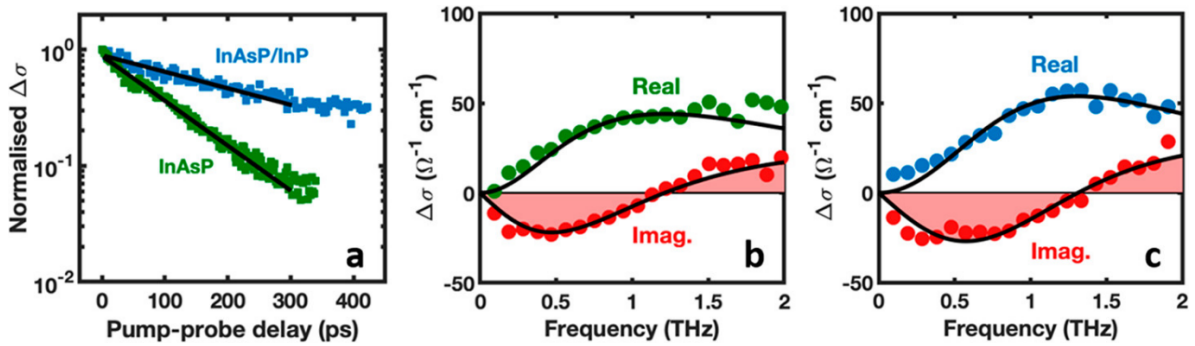

Figure 1: Influence of the InP surface passivation layer on carrier dynamics probed by OPTP measurements. (a) Normalized photoconductivity decays of InAsP and InAsP/InP nanowires on a semilogarithmic scale. Photoconductivity spectra of (b) InAsP and (c) InAsP/InP nanowires at a delay of 10 ps after photoexcitation. [1]

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