SOFI Showcase 2024 – Abstracts

Invited Speakers

Dr David Fairhurst (University of Edinburgh) - The Ouzo effect: adding a splash of dynamics to the Water/Ethanol/Oil phase diagram

Ouzo is a colorless aniseed-flavour liquor which turns cloudy when diluted with water. This process, known as *spontaneous emulsification*, occurs as the added water dilutes the ethanol, leading to precipitation of oil-rich microdroplets. Despite much work on the dynamics of this process, the full equilibrium phase diagram for water-ethanol-anise oil has not previously been determined experimentally. We present data determining the two-phase region and the spinodal curve separating unstable from metastable behaviour. We also measure the composition of coexisting phases, indicated on the phase diagram by tie lines, identify the plait point (critical point) and determine densities and surface tensions of coexisting phases. We then use this equilibrium data to better understand spontaneous emulsification and other complex dissolution dynamics.

Dr Dipa Roy (University of Edinburgh) - Sustainable Composites - Challenges and Opportunities

Student Talks

Serena Berberolli (University of Leeds)- Investigating gut microbiota-mucus interactions within an engineered colonic simulator

The colonisation of the gastrointestinal mucosal layer by the gut microbiota and the interaction of commensal bacteria with mucins play a fundamental role in regulating host homeostasis and disease susceptibility. However, the limitations of current *in vitro* models pose a challenge to deepening our understanding of the dynamics of microbial populations in a physiologically representative context. The aim of this study was to evaluate the role of a mucus coating in MiGut[1], an innovative engineered simulator of the colonic environment, on mucus-utilising microbial communities. To this end, 3D printed scaffolds designed to support gut relevant biofilm formation were coated with a mucus mimetic hydrogel and placed into the vessels of the MiGut platform. Through precise regulation of pH and temperature, and the continuous bubbling of nitrogen to uphold an anaerobic environment, it is possible to culture gut bacteria in a context that closely represents physiological conditions in the human colon.

A spatiotemporal analysis was conducted by sampling different modelled sections of the colon within MiGut[1] at different time points. A total of ten different mucosal bacterial species were quantified via qPCR, including *Akkermansia.* Our results showed a notable increase in biofilm formation on mucus-coated scaffolds vs untreated scaffolds, highlighting the pivotal role of mucin in promoting bacterial adhesion and colonisation, and in shaping the microbial composition in the colonic environment. This included significant increases in *Akkermansia* spp. (6,01 log10 $\log_{10}$ CFU/mL) and *Bifidobacterium* spp. (8.72 $\log_{10}$ CFU/mL) on the mucus coating vs plain coated biofilms (4.90 $\log_{10}$ CFU/mL and 7.04 $\log_{10}$ CFU/mL respectively).

These findings obtained from this optimized model contribute to an improved understanding of the gut microbial ecology, paving the way for more complex studies that aim to evaluate the effect of exogenous factors on mucus-associated species and, ultimately, develop strategies to improve gastrointestinal health.

1. Davis Birch WA, Moura IB, Ewin DJ, et al. MiGut: A scalable in vitro platform for simulating the human gut microbiome—Development, validation and simulation of antibiotic-induced dysbiosis. *Microb Biotechnol*. 2023.

Co-authors:
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Holly Bridge (University of Edinburgh) - Dense Suspensions of Rods: Mechanisms of Curvature-Dependent Jamming

Dense suspensions are a broad class of out-of-equilibrium systems that often display interesting macroscopic behaviour under flow. The rich physics observed for suspensions of spheres can be expanded to particles of more complex geometries, resulting in novel flow phenomena. This work applies concepts from dry granular physics to model the rheology of suspensions of curved rods in LAMMPS. Specifically, we investigate the interplay between rod curvature (exploring an angular range of 0-2π) and microstructural properties. In our sheared suspensions, we probe the shape-dependent jamming transition whereby, the jamming volume fraction is found to be a non-monotonic function of curvature. Using Q-Tensor theory, we show alignment with the flow field and consequent arising orientational order contributes to the different packing abilities of rods, arches and disks.

Co-authors: Holly Bridge, Tyler Shendruk, Christopher Ness, Gavin Melaugh

Benjamin Devenish (Durham University) - From Tip to Ship: Characterisation of New Marine Antifouling Coatings

Biofouling is a well documented problem on marine structures, such as offshore platforms and large shipping vessels. Fouling of these surfaces can increase costs as well as reduce the operational lifetime of structures[1], both major issues in marine industries. Current antifouling strategies rely on biocides, such as cuprous oxides, which kill fouling organisms coming in close contact with the coated surfaces during the early stages of biofouling[2]. While effective, this method is known to have detrimental impacts on marine ecology, especially in busy water ways[3]. There is thus a need for new, novel antifouling strategies that do not rely on biocides. One possible solution entails physical methods, whereby the function of the antifouling coating comes from the inability of fouling organisms to attach to the protected surface due to its mechanical and physical properties, such as low surface energies and water contact angles[4]. However, most existing strategies cannot easily be scaled up for routine use in shipping or marine industries. In this research, we investigate a promising new strategy for a polymer-based antifouling coating that combines particular mechanical properties together with nanoscale control of the surface hydrophobicity. This strategy can easily be scaled up, however its specific mode of action and evolution with aging are not yet fully understood. Using Atomic Force Microscopy (AFM) in solution, we characterise differences between candidate coatings, quantifying nanoscale structural and viscoelastic properties that we aim to correlate with the coatings' antifouling performance. These results form a platform for the rational development of functional antifouling strategies to be deployed on a larger scale.

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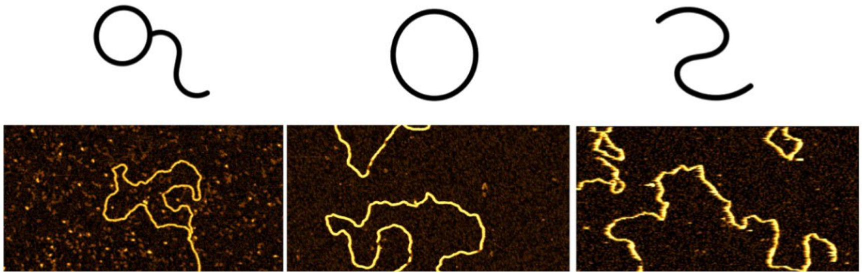
Co-authors: Professor Kislon Voitchovsky (Durham University), Robin Heath (AkzoNobel, Gateshead)

Jennifer Harnett (University of Edinburgh) - Folding and Sticking: How DNA Origami's Sticky Interactions Dominate Topological Effects in Rheology

Fundamental properties of DNA-based materials, including DNA sequence, length, topology, and external factors such as ionic strength and temperature, collectively influence their properties. However, how these factors influence the material properties of highly concentrated DNA solutions have remained largely unexplored. In this talk, I will present our work investigating how the microscopic topology of DNA influences the macroscopic material properties of the solution.

DNA can be 'folded' into virtually any arbitrary design by combining a single stranded scaffold DNA with many smaller staple strands in a technique known as 'DNA origami' [1]. We use this technique to create a linear, circular and tadpole design of DNA origami, then concentrate to create an entangled solution of DNA. The viscoelastic properties are investigated using microrheology. Each topology is expected to form unique entanglements at high concentrations. Simulations predict that tadpole polymers will significantly differ from linear and circular polymers due to topological constraints or 'threadings' between the polymers [2].

Surprisingly, we find that the DNA topology is not the dominating factor influencing the rheological properties of DNA origami, but instead presence of short-lived bridging interactions between the DNA strands mediated by the 'staples'. The linear topology deviates from the expected 'reptation model' of linear polymers, and we find instead that the linear DNA origami construct agrees with a 'sticky reptation model' [3].



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Co-authors: Dr Davide Michieletto

Bianca Hazt (University of Leeds) - Effect of thermal treatment on lactoferrin: unveiling insights for mucoadhesion

There is an increasing demand for biocompatible materials capable of assisting in the localized delivery of agents. Mucoadhesives appear as promising candidates in this area, as they promote an extended contact time between materials and soft mucosal layers, also offering the possibility of coating and protecting damaged tissues. In this work, we hypothesize that lactoferrin (LF), a milk protein, can act as such and that thermal processing affects its mucoadhesive performance. To evaluate this, we employ a combination of techniques including rheology and quartz crystal microbalance with dissipation monitoring (QCM-D). Results show that post-denaturation, the viscosity of lactoferrin remains unchanged and a shear-thinning behavior at concentrations as low as 0.5 wt% arises from interfacial contribution effects. There is an enhancement in the viscosity values of mucin and lactoferrin mixtures (at 0.5 wt.% each) when comparing them to those of the individual components. These increased viscosity values for lactoferrin-mucin complexes unveil the rheological synergism usually associated with mucoadhesive materials, as even at these low concentrations the interactions between mucin and LF lead to the formation of larger structures. The adsorption behavior of LF onto mucin was monitored using QCM-D measurements, which confirmed that the denatured forms of lactoferrin adsorbs to mucin at a larger extent, compared to its native form. This heightened mucoadhesivity of the denatured form of the protein is attributed to its positive surface charge and surface hydrophobicity, as no free thiols were detected. By tuning the extent at which lactoferrin is denatured, it is possible to control the assembly with mucin, paving the way for novel designed protein-based mucoadhesives.

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Co-authors**:** Daniel Read, Oliver Harlen, Wilson Poon, Adam O’Connell, Anwesha Sarkar*

Megan Holdstock (University of Leeds) - The Impact of Insoluble Particles on the Rheology and Structure of Edible Fats

Controlling the dispersion of solids in non-aqueous media such as oils poses a considerable challenge, particularly when the particle is amphiphilic in nature. This work has set out to develop a better understanding of such materials in the context of a filled fatty matrix: chocolate with added insoluble plant protein particles. In this application, both texture and crystallization properties are crucial in formulating products that meet consumer expectations.

The dispersion behaviour of such plant protein particles in oil was studied using rheological techniques and compared to a model colloidal system; silica nanoparticles with known surface chemistry. Mechanical treatment was used to reduce the inherently large size of protein particles to submicron range, ensuring a desirable mouthfeel. Protein particles formed tightly bound aggregates which were poorly wetted by oil and had minimal effect on the viscosity of the system, whereas low (< 1 vol.%) volume fractions of silica particles increased the viscosity considerably. Small- and wide-angle x-ray scattering were employed to determine the effect of these colloidal particles on the crystallization properties of cocoa butter. The crystal structure of cocoa butter polymorphs were unchanged by the addition of both particle types, indicating that they remain in the fluid phase and do not integrate into the crystal structures. Oscillatory rheology was also used to probe the temporal evolution of isothermal cocoa butter crystallization and evaluate the effect of particles on fat crystal networks. Comparison of these systems shows that the dispersion behaviour of the two particle types in oil differs, likely due to differences in particle size and surface chemistry. These findings were applied to more complex multi-particle confectionary systems with the aim of creating a material with desirable texture and melting attributes.

Co-authors: Professor Brent Murray, Professor Anwesha Sarkar, Professor Michael Rappolt and Dr Paraskevi Paximada (all School of Food Science & Nutrition, University of Leeds) & Dr. Isabel Celigueta Torres, and Dr. Hugh Powell (Nestlé PTC, York)

Vinay Kopnar (Durham University) - How does synergy play a role in the mechanics of a double-network hydrogels?

Composite materials are found almost everywhere in nature. The synergistic effect of collagen which is good at absorbing and dissipating energy but is highly inextensible, and elastin which is extensible but very poor at dissipating energy help tendons in our body transfer force from muscles to bone structure. For this reason, composite polymeric materials present a useful model system for understanding the mechanical synergy exhibited in living materials. Of particular note are hybrid double-network (DN) hydrogels[1] that contain two interpenetrating polymer networks dispersed in water, one of which is transiently crosslinked through noncovalent interactions and the second of which is permanently crosslinked through covalent interactions. They exhibit enhanced toughness which is governed by yielding transition[2]. Despite the apparent importance of yielding process in hybrid double-network hydrogels, it remains challenging to precisely identify the yielding point, to quantify the structural changes that take place during yielding, and to examine how this process relates to the intermolecular interactions between the two networks.

Through this presentation, we demonstrate how individual networks play out their role in determining the non-linear properties of a DN hydrogel. We illustrate a way to disrupt links between the two networks and thus, present the synergistic effect caused by these links on the linear properties as well as the failure mechanics of the DN hydrogel. Simultaneously, we present how Large Amplitude Oscillatory Shear (LAOS) rheology[3] in conjunction with systematic design approach could help in studying structure-property relationship of such composite materials.

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Mahya Mehari (University of Edinburgh) - The interplay between topography and contact line pinning mechanisms on flat and superhydrophobic surfaces

Sliding droplets are of practical importance in various applications from water harvesting to self-cleaning surfaces. The onset of the droplet motion can, in the first step, be simplified to the initial displacement of the front and back contact lines of a two-dimensional droplet. To move a three-phase contact line, a de-pinning force needs to be applied, where the amount of that force depends on both surface chemistry and topography. However, a unified understanding and description of the de-pinning force on both flat and superhydrophobic surfaces is still lacking. Aiming to bridge the existing gap in our understanding of the three-phase contact line pinning on flat and microstructured superhydrophobic surfaces, our findings indicate that a general model, based on two different pinning mechanisms, can describe the pinning force on both flat and microstructured surfaces. We compare the general model against experimental data from literature, as well as our experiments on flat and microstructured surfaces coated with a liquid-like layer of grafted polymer chains. While this theoretical framework can be useful for designing micro-engineered surfaces on which the contact line behaviour is important, it also provides a potential experimental strategy to distinguish the contribution of defects from that of molecular re-orientation to contact line pinning on a given solid material. Having a description of the phenomena resisting the beginning of the droplet motion leads to new questions about the behaviour of a moving droplet in the very initial stage of its motion.

Co-authors: Camelia Dunare, Khellil Sefiane, Simon Titmuss, Job H. J. Thijssen

Will Ogle (University of Leeds) - DCM Alternatives for use in Steglich Esterifications, for Green and Sustainable Liquid Crystal Syntheses

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The Montreal Protocol (1989) banned carbon tetrachloride as a solvent due to its ozone depleting properties and was largely replaced by dichloromethane (DCM).[1] Halogenated solvents must now be phased out. DCM is hepatotoxic, neurotoxic, carcinogenic and the cause of at least 85 deaths from 1980 through acute exposure. [2–5] Moreover, it has been shown to damage the ozone layer,[1,5] hence, the US EPA have proposed a ban. DCM needs to be urgently replaced with less hazardous solvents, according to the ACS Green Chemistry Institute Pharmaceutical Roundtable.[5]

We screened twenty green and sustainable solvents to find the most efficacious DCM alternative for the synthesis of ester groups in a typical liquid crystal such as CZP-5-N.[6] Several factors are considered: yield, safety, health, and environmental impact (SHE). For each solvent we performed the synthsis of CZP-5-N on mmol scale using EDC.HCl in a Steglich esterifiaction. Reactions were performed four times, to give the indicated yield. The SHE scores were obtained from the CHEM21 and GSK solvent selection guides, [7,8] and normalised to get compariable data. The best performing solvent (dimethyl carbonate) was then used in the synthesis of other common liquid crystal substrates, giving excellent results, even for electron poor phenols. Esters are highly prevalent in the new ferroelectric nematic phase, due to their role in polar conjugation.[9] Therefore, sustainability in this area is crucial for the next generation of liquid crystal materials, such as RM734, DIO and their analogues.

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Saabir Petker (University of Edinburgh) - A Molecular Dynamics Study Towards Barocaloric Polymer Simulations

Current refrigeration processes consume over 20% of the global energy usage and emit high global warming potential gases. [1] This is an unsustainable practice, so new refrigerants must be implemented 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 focusses 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 work on barocaloric polymers, and fewer computational work, so the exact origins of their large BCEs are unknown. [6] The BCE in polymers is affected by the glass transition temperature (T_g), below which the polymer is in a glass state and above which the polymer is considered a rubber. Below T_g there are low adiabatic temperature changes (ΔT_{ad}), and when pressurising above T_g, ΔT_{ad} increases drastically. We explore the glass transition and its effect on the BCE in NBR using molecular dynamics simulations.

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Toby Read (University of Leeds) - Rapid and Robust Living Anionic Polymerization Screening using an Automated flow reactor

The power of living anionic polymerisation (LAP) in flow is yet to be fully utilised. In literature, LAP in flow has explored changes to the reactor platform, polymerising a range of monomers to make homopolymers and copolymers, and using THF to speed up the reaction rate.[1–3] However, unlike flow reactors for RAFT polymerisation, the literature for LAP in flow does not take advantage of some key benefits of flow chemistry such as automation.[4–6] Herein we use an automated flow reactor with inline gel permeation chromatography (GPC) to rapidly screen a range of residence times and temperatures for the LAP of styrene, isoprene and myrcene. This allows trends in molecular weight and dispersity to be observed with ease. The reactor conditions, screened using a central composite design of experiments, approximates the ideal total flow rate and temperature for a given monomer. We demonstrated that the LAP of styrene reaches 100% conversion at relatively short residence times and low temperatures, while the LAP of isoprene requires higher temperatures and longer residence times to produce significant polymerisation. This methodology screens monomers faster than batch LAP reactions, allowing greater consistency in the conditions between reaction points and opening the door to more automated flow processes with LAP.

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Martin Screen (Durham University) - Crystallising Proteolysis Targeting Chimeras

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Targeted protein degradation (TPD) is an emerging therapeutic modality with the potential to tackle disease-causing proteins previously deemed "undruggable" with conventional small molecules. In the 20 years since the conception of a proteolysis targeting chimera (PROTAC), a molecule capable of harnessing the ubiquitin-proteasome system to degrade a target protein, TPD has moved from academia to industry and is attracting substantial interest, with more than 10 PROTACs now in clinical trials.[1] However, PROTACs are very poorly water-soluble and face challenges regarding their development into drug products with sufficient bioavailability. Formulation strategies successfully employed for other poorly water-soluble small-molecule pharmaceuticals may help to improve their bioavailability by increasing their solubility and/or dissolution rate.[2] Pre-formulation studies are required first to understand the physicochemical properties of PROTACs before any such strategies can be implemented, since there is very little literature in the nascent field of PROTACs formulation.[2] Understanding the role non-covalent interactions have on both crystal packing and aggregation in solution is an important step for implementing various formulation strategies. We are currently investigating the crystallisability, stabilisation of amorphous solid forms, formation of cocrystalline and coamorphous solids of a cereblon PROTAC and a set of structurally similar compounds.

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Ke Sun (Durham University) - Nanoparticle adhesion at liquid interfaces

Particle adhesion at liquid interfaces is crucial for wide-ranging applications, including drug delivery and surface cleaning [1, 2]. With the rise of nanotechnology, nanoparticles have gained interest due to their increased surface area and enhanced mobility. However, previous studies have mainly focused on micron- or millimetre-sized particles [3, 4], leaving nanoscale phenomena less understood. In this study, we combine Atomic Force Microscopy (AFM) and continuum simulations to investigate the details of nanoparticle adhesion at liquid interfaces, considering the interfacial energy, particle geometry, and line tension (Figure 1). AFM allows us to precisely measure nanoparticle adhesion forces, with the AFM tip simulating a nanoparticle. Computationally, the Surface Evolver [5] is used to visualise the interface and quantify the adhesion energy. Our experimental and simulation results agree quantitatively, demonstrating that continuum thermodynamics concepts remain applicable down to the nanoscale. We find that nanoparticle adhesion is primarily controlled by surface tension, with the particle's geometry and the liquid contact angle determining the magnitude of the adhesion force and the shape of the force profile. Moreover, this model can be further expanded to include additional complexities, such as imperfect geometries and heterogeneous surfaces. These insights address existing knowledge gaps at the nanoscale and will benefit the development of new technologies involving functional nanoparticles and smart interfaces.

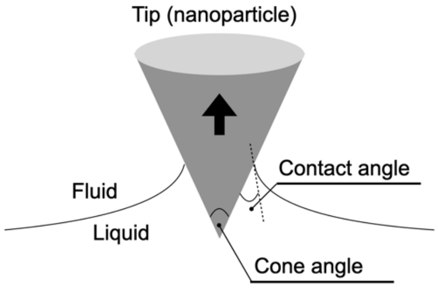

Figure 1: Sketch of a nanoparticle at a liquid interface.

Co-authors: Yonas Gizaw, Halim Kusumaatmaja, and Kislon Voïtchovsky

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Jinyi Xuan (Durham University) - Acid-Base Switchable Synthetic Small Molecule Walkers

Molecular walkers found in biological systems are highly processive, repetitive, and able to walk directionally with high degrees of control. Motor proteins, such as kinesins, can walk down a track whilst carrying out cellular functions. Synthetic small molecule walkers have been designed to mimic the walking behaviour using dynamic covalent chemistry. We employed the dynamic nature of Smiles rearrangements to create switchable molecular walkers. To build the 5-step walker, the walking group was initially loaded on to the loading site, then walked to the terminal position in an autonomous and reversible fashion. The positional switch in intramolecular rearrangement of the walking group on the 5-step track was achieved by alternating base and acid conditions. Both the loading position and the terminal position walker molecules were successfully isolated; and structures confirmed with X-ray crystallography. ^{1}H NMR was used to monitor the walking behaviour, and results confirmed that an excellent positional control was achieved. A ratchet mechanism was explored and installed in a 3-foothold walker. ^{1}H NMR experiments demonstrated the directional walking behaviour. Ultimately, we hope to further optimise and exploit Smiles Rearrangements in the construction of longer or directional walkers.

Co-authors: L. M. P. Ter-Ovanessian, S. Vijayakarishnan, M. O. Kitching.*

Poster Abstracts

Daisy Akgonullu (University of Leeds) - Interfacial behaviour of potato protein microgels: Role of pH and interface type

Microgels are deformable particles of cross-linked solvated polymers, which have tuneable viscoelasticity within bulk media and the ability to act as Pickering stabilisers at interfaces[1]. This study focuses on understanding the interfacial performance of potato protein microgels (PoPM) in comparison to un-gelled potato protein (PoP). Potato protein (PoP) was used to produce microgels of sub-micron diameter via a top-down approach of thermal crosslinking followed by high-shear homogenisation of the bulk gel.

Although, both PoP and PoPM show surface activity, it was demonstrated that the behaviour of PoPM monolayers may not be as viscoelastic as those of PoP. Monolayer viscoelasticity is a key parameter in determining emulsion stability as it indicates a greater capacity for the maintenance of the stabilisers' functionality at oil-water or air-water interfaces. To explore means of facilitating the development of viscoelastic monolayers formed from PoPM and assess their response against PoP, interfacial shear rheology was conducted under varying conditions: to assess the influence of the polarity of the oil used to form the interface (tetradecane *cf.* 1-octanol) and that of the subphase pH (pH 3 *cf.* pH 7).

Interestingly, despite reaching a plateau in interfacial storage and loss moduli (G_i', G_i'') at quicker rates when in conditions of pH 3 and the 1-octanol-water interface, PoP reached highest G_i' and G_i'' in an environment of pH 7 and tetradecane-water interface. Meanwhile, PoPM reached highest G_i' and G_i'' under acidic conditions, which implies that a lower pH may aid in optimising their compact structure to increase interfacial interactions.

These results show that both pH and oil polarity offer means of tailoring microgel interfacial elasticity. Thus process-induced tuning of potato protein-based microgels may offer a new sustainable platform for the development of responsive Pickering emulsions to tackle a range of industrial challenges.

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Aqib Asif (University of Edinburgh) - Understanding the Mechanisms of self-cleaning surfaces

Maintaining cleanliness is crucial in various industrial processes and engineered surfaces, yet the economic and ecological burdens of using sanitizing solutions present significant challenges in the journey toward a net-zero world. This has sparked interest in self-cleaning surfaces inspired by nature. For example, droplets on superhydrophobic surfaces (SHS), modelled after the lotus leaf, have high mobility and dirt is lifted off as the droplet rolls. On the lotus leaf, which has inspired a class of biomimetic surfaces known as superhydrophobic surfaces (SHS) (Fig.1a), a droplet has high mobility and dirt is lifted off the surface as the droplet rolls. Two alternate approaches are creating liquid-infused surfaces (LIS) by imbibing the surface with oil (Fig.1b) [2,3], and omniphobic liquid-like surfaces (LLS) by covalently grafting polymers to achieve liquid repellency (Fig.1c) [4].

In addition to being applicable to self-cleaning, SHS, LIS, and LLS are commonly studied for their anti bio-fouling and anti-icing properties. Therefore, it is crucial to have design principles which guide how to create these surfaces so they resist particle contaminants. However, a lack of understanding of the mechanisms driving self-cleaning means trial and error is still the prevalent approach to fabricating such surfaces. To address this, we investigate the forces involved in contaminant removal on SHS, LIS, and LLS, focusing on rigid particles and more complex contaminants like food with non-Newtonian rheology. This will be achieved by using a combination of Lattice Boltzmann Method simulations and innovative experimental setups to measure friction forces and viscous dissipation during droplet movement on these surfaces.

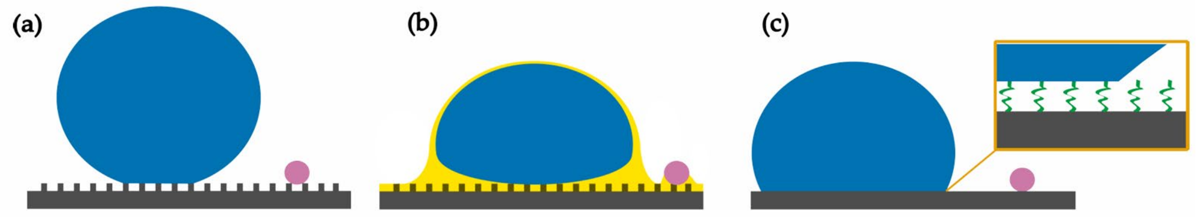

Figure 1: Schematics of droplet (blue) and contaminant (pink) on different surfaces: (a) superhydrophobic surface (SHS), (b) liquid-infused surface (LIS), and (c) omniphobic, liquid-like surface (LLS). The inset shows the nanoscopic structure.

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James R Austin (University of Leeds) - Thermal Analysis and Characterisation of RAFT-Synthesised PMA Vitrimer Precursors of Varying Molecular Weights

Thermal analytical techniques have shown themselves to be versatile tools used to analyse the structural properties of a variety of materials and architecture. Differential Scanning Calorimetry (DSC) relates the heat capacity of a material to its intrinsic dynamics as the material relaxes and undergoes conformational changes [1]. Through this, it is possible to glimpse the behaviour of glassy materials in and around the glass transition or as they begin to flow. Thermogravimetric Analysis (TGA) characterises the weight of a material as a function of temperature or time under prolonged heating ay high temperatures [2], providing information on the composition and the thermal stability of the material as well as observations of the physical processes that may occur such as sublimation, vaporization, and desorption.

Recent work has utilised DSC and TGA to determine the thermal stability and characterise the glass transition of a series of RAFT-synthesised poly(methyl acrylate) polymers of differing molecular weights, which are precursors to a set of boronic ester based vitrimers [3]. The variation in their properties is discussed in relation to the changes in these precursors' molecular weights. An understanding of the baseline behaviour and dynamics of these simple systems allows for easier observations of the effects when modifying these systems, such as via copolymerisation or including cross-linking functionality.

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Guanyi Chen (University of Leeds) - All-cellulose composite made in a DMSO/IL/Water ternary solvent system

An all-cellulose composite (ACC) is a composite that uses cellulose as both its reinforcement fibres and matrix (Huber et al., 2012). It is a material that has a high potential to replace commercial fossil fuel-based plastics. Cellulose is a renewable natural biopolymer consisting of a chain of glucose molecules joined by β-1,4- glycosidic linkages (Guerriero et al., 2016). ACC is also a green composite because it is a composite of natural fibres and biopolymers with no chemical incompatibility between reinforcement fibres and the matrix (Huber et al., 2012), meaning that the recycling process of ACC is simplified. Cellulose dissolution is a step in the production of ACC achieved by the disruption of intra- and inter-hydrogen bonding of cellulose molecules (Sun et al., 2009). Ionic liquids (ILs) and its co-solvent like dimethyl sulfoxide (DMSO), are often used for cellulose dissolution. It has been reviewed in the literature that water decreases the cellulose dissolution rate through the competitive hydrogen bonding with cellulose, therefore addition/contact of water in cellulose dissolution needs to be avoided. However, the presence of water in the DMSO/IL solvent system is inevitable, i.e. through atmospheric moisture (Paiva et al., 2022). To achieve an industrial-level production of ACCs, the issue of water sensitivity in cellulose dissolution needs to be resolved.

In a recent study, it has been found that water will not decrease the cellulose dissolution rate but cooperate with the DMSO/IL solvent system if its molar concentration in the DMSO/IL solvent system is below 0.40. The authors studied the cellulose dissolution in a DMSO/IL/Water ternary system, using nanocellulose and cellobiose (a short repeat unit of cellulose). Here, we studied the mechanical properties of ACCs made in a DMSO/IL/Water ternary system and provided some preliminary results and suggestions.

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Naomi Crabbe (Durham University) - Small Peptide-analog Hydrogelators: From Synthesis to Application

Low molecular weight gelators (LMWGs) that undergo self-assembly have been extensively investigated for numerous biomedical applications owing to their facile synthesis and tunability, low cost, and biocompatibility[1][2][3][4][5]. Among these, Fmoc-FF (9-*N*-fluorenylmethoxycarbonyl-diphenylalanine) has been the most widely studied model supramolecular hydrogel system, attributed to its rapid self-assembly in response to various stimuli[6]. Much has been revealed about the self-assembly properties of peptides such as Fmoc-FF, but they possess an underlying disadvantage of susceptibility to proteolysis *in vivo*[7]. This proteolysis results in low bioavailability, and limits their potential use in biomedical applications.

N-substituted glycine oligomers, or peptoids, are compounds that mimic peptide behaviour while offering enhanced stability against enzymatic and proteolytic degradation[7]. The fluorenyl and phenyl functionalities in Fmoc-FF contribute significantly to hydrophobic and p-p interactions, which are crucial for gelation and gel strength, while hydrogen bonding along the peptide backbone plays a less prominent role[8] [9]. Recent findings have shown that similar design principles may also be important in the gelation of *N*-benzyl glycine substituted Fmoc-FF derivatives[10]. This work aims to demonstrate the straightforward synthesis of Fmoc-FF inspired LMWGs and discuss the design considerations, characterisation methods across multiple lengthscales, and potential applications of these systems.

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James Andrew King (University of Leeds) - Dissolution Behaviours of Cellulose and Silk Fibroin in 1-ethyl-methylimidazolium Acetate and Dimethyl Sulfoxide and Processing for Hybrid Films

Hybrid biopolymer materials could help combat growing issues with plastic pollution, but processing and dissolving these polymers remains a challenge. 1-ethyl-3-methylimidazolium acetate (EmimAc) is a promising eco-friendly solvent but suffers from high viscosity limiting effective dissolution. Dimethyl sulfoxide (DMSO) has been proposed as a cosolvent and shown to reduce viscosity and improve dissolution speed with equivalent solvent thermodynamic quality at up to 50 wt %. However, dissolution behaviours for biopolymer blends and in typical processing conditions remain unexplored for this solvent system. Here we report rapid dissolution and maintained solvent thermodynamic quality up to 80 wt % DMSO for microcrystalline cellulose at 100 °C, while unprocessed silk fibers dissolve more quickly at higher EmimAc concentrations. We show that macroscopic dissolution stops before molecular level saturation is achieved by comparison of nuclear magnetic resonance, rheological data, and optical microscopy. Our findings explain discrepancies in literature solvent composition optimums and help to improve understanding of biopolymer dissolution. Lastly, blend solutions are used to prepare hybrid films indicating how this work may provide a foundation for effective solvent choice in future biocomposite studies.

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Josh Mckeown (Durham University) - Carbonara: Rapid SAXS-Based Refinement of Predicted Protein Structures

While AI-based tools like AlphaFold have revolutionised protein structure prediction, these static models often fail to capture the dynamic nature of proteins in their native environment. Small-angle X-ray scattering (SAXS) offers valuable insights into protein shape and conformational changes under near-native conditions. However, interpreting this low-resolution data remains challenging due to the rotational averaging proteins undergo while tumbling in solution, leading to many non-unique and often physically unrealistic structural interpretations.

We present Carbonara, a novel computational method that narrows the vast conformational space by combining AI predictions with SAXS data. Our approach uses a coarse-grain protein representation of alpha carbon atom positions to describe a discrete geometric curve. This allows us to enforce mathematical bounds that promote (but not guarantee!) physical realism on generated structures while remaining computationally efficient. Consequently, we can quickly and efficiently search a protein's conformational space to find physically viable structures that agree with the experimental SAXS profile.

Carbonara's flexibility is a key strength, accommodating a wide range of scenarios and prior information. Our method can handle multiple conformational states, multimeric assemblies, and incorporate experimentally derived inter- and intra-molecular distance constraints. This versatility not only further narrows the conformational search space but also enables us to generate more accurate and biologically relevant predictions. By integrating diverse sources of information, Carbonara provides a comprehensive approach to structure refinement that adapts to the complexity of real-world protein dynamics.

We demonstrate Carbonara's utility in refining AlphaFold-predicted structures and characterising proteins with multiple known states, potentially revealing functionally relevant conformations not captured by static structural predictions. This approach bridges the gap between crystallographic and AI-generated models and experimental in-solution SAXS data, offering a powerful tool for refining and validating protein structures in near-native conditions.

Carbonara's impact extends across structural biology and drug discovery, offering insights into protein dynamics and enhancing structure-based design. By accurately representing proteins in their native states, it advances our understanding of protein function and interactions under biologically relevant conditions.

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Niamh O’Donoghue (University of Leeds) - Development of Lyotropic Liquid Crystalline Nanoparticles for biomedical applications

Development of successful drug candidates is often impeded by poor biocompatibility and bioavailability. Lyotropic liquid crystalline systems have gained popularity both in academic research and clinically as an effort to surmount these hindrances. Liquid crystalline nanoparticles (LCNPs) are non-lamellar lipid nanoparticles which are composed of often FDA-approved materials such as amphiphilic lipids and offer solubilisation of hydrophilic and hydrophobic cargo.

To understand the biocompatibility of these LCNPs, we have investigated the factors that define their intrinsic cytotoxicity and cellular uptake. Three ternary lipid systems of different lipid nature, composition and nanostructure were designed and analysed using Small Angle X-ray Scattering (SAXS) and Dynamic Light Scattering (DLS). Different nanostructures including cubosomes, hexasomes and Fd3m micellosomes have been revealed at different lipid compositions and these have been assessed for their in vitro toxicity using cell viability assays, and cellular uptake using fluorescence microscopy and flow cytometry. This work reveals that lipid nature/ chemistry is primarily important in design of biocompatible LCNPs, with nuances in nanostructure also identified. This gives insight and contributes to a framework for design of these particles for delivery applications in the future.

To gain further insight, we aim to encapsulate and monitor in vitro release of model hydrophobic drug from these nanoparticles. By monitoring any change in internal structure during these processes, our objective is to identify if nanostructure/ delivery vehicle properties and release rate of hydrophobic drug are linked for these systems.

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Ruairí Phelan (University of Edinburgh) - Extending the Vicsek model to include hydrodynamic interactions

Collective motion is found everywhere in nature, whether that be flocks of birds, schools of fish, or suspensions of swimming bacteria. In recent decades, it has also been extensively studied by scientists as an example of an "active matter" phenomenon that breaks much of the intuition we might carry over from traditional soft matter physics. The most famous mathematical model for this was proposed by Vicsek et al. in 1995[1], with point particles that move at constant speed and align with their neighbours, while experiencing fluctuations in their orientation. This simple model lends itself to analytical study, while still capturing the behaviour of a whole class of systems.

We build upon an extension to this model [2] to investigate its applicability to microswimmers in a background fluid: first introducing the "run-and-tumble" motion found in bacteria, and then adding in hydrodynamic interactions between particles. By comparing simulations of the "dry" and "wet" models, we can identify if it still falls under the Vicsek universality class, or whether there is a new fundamental change in behaviour.

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Ofelia Popescu (University of Edinburgh) - The Role of Filamentation in E. coli Survival in Microfluidic Droplets Treated with β-lactam Antibiotics

Escherichia coli's ability to survive β-lactam antibiotics (like ampicillin), is crucial for understanding bacterial persistence and resistance mechanisms. At low concentrations of ampicillin, we observe a striking increase in filamentation, a morphological response where cells elongate without division. Our objective is to investigate the role of filamentation in bacterial survival under antibiotic stress.

In this study, we explore the dynamics of E. coli populations treated with ampicillin inside microfluidic droplets, allowing us to generate high through put data in independent growth environments. The image analysis allows us to observe growth patterns of these populations identifying both common and rare events within the droplets.

Key questions:

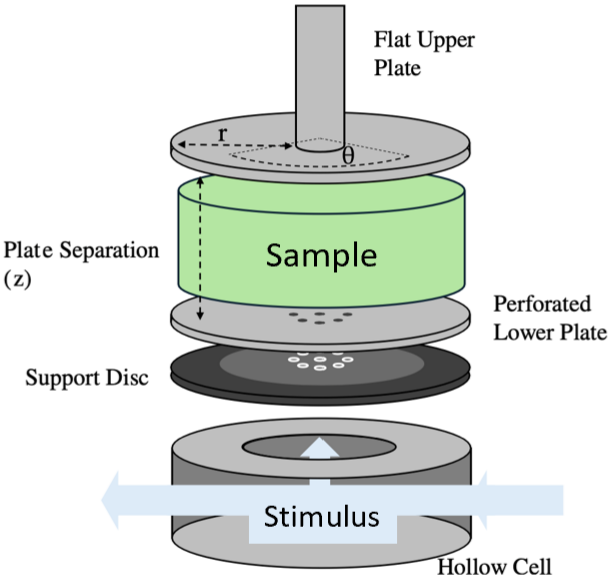
Is filamentation essential to survival? Is filamentation dependent on the initial population size? What is the average length of bacteria at the time of resurrection (i.e. restarting division)?

Qandeel Saleem (Durham University) - Rheodialysis: Exploring Real-Time Gelation Kinetics in Diverse Polymer Networks

This study introduces **Rheodialysis**, a novel experimental platform that enables real-time monitoring of gelation kinetics in fast-gelling polymer systems, addressing key challenges in fields such as biofabrication, food science, and tissue engineering. Traditional ex-situ rheological methods are limited in capturing the rapid and dynamic crosslinking events due to their closed-system nature. These rapid kinetics are difficult to observe without disturbing the fragile gel structure during rheometer sample loading. Our customized setup overcomes these limitations by allowing simultaneous rheological measurement and manipulation of the sample's chemical environment, making it ideal for studying fast gelation processes.

As a proof-of-concept, we used Rheodialysis to investigate the gelation of alginate in the presence of calcium ions, focusing on the rapid diffusion and crosslinking events that occur within 0.1–1 second. This setup, comprising a parallel-plate geometry with an in-house designed rheo-dialysis cell, allows calcium ions to diffuse through a semi-permeable membrane into the alginate sample, enabling precise control over the ion diffusion length and gelation kinetics and offering new insights into how varying diffusion lengths, controlled by adjusting the distance between the rheometer plates, influence crosslinking density and gel structure.

Currently, we are extending the platform to mimic fibrin clot formation in the presence of thrombin, a critical process in blood coagulation. By studying the interaction between mechanical shear and enzymatic activity during clotting, we aim to provide a more comprehensive understanding of fibrin network formation, with significant implications for both biomedical applications and the study of clotting disorders. Overall, Rheodialysis offers a powerful tool for exploring diverse gelation mechanisms, providing real-time data on the structural evolution of soft materials under both chemical and mechanical stimuli.



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Ella Sapsford (University of Edinburgh) - CrysDoS Gels and the Effect of End Group on the Rheology of Polypseudorotaxanes

Mechanically interlocked structures, common in nature, offer novel properties but are hard to synthesize and scale. [1] Rotaxanes, perhaps the simplest interlocked structures, consist of a ring threaded on an axle, with polyrotaxanes (PRs) made by threading polymeric guests in cyclic hosts. Most commonly poly(ethylene glycol) (PEG) and cyclodextrin (CD) are commonly used for this.[2] Cyclodextrin are cyclic sugar molecules and come in three commercial homologues: α-, β-, and γ-CD; which have an increasing cavity diameter respectively. As a sugar derivative the CD have hydroxy groups on both faces which are strongly hydrogen-bonding; CD, therefore, readily crystalise. Where threaded CD therefore form microcrystalline domains that act as crosslinks,[3] or cause the polymers to aggregate.[4] End-group modification of PEG, such as PEG(Azo)2, forms elastic gels in comparison to unfunctionalised PEG with instead forms only a viscoelastic fluid. The significantly increased plateau *G'* with unmodified PEG is due to 'bridging' effects, resulting from the distribution of CD at the chain ends.

Without CD-CD interactions, no crystalline domains form, leading to lower plateau values. When copolymerised with hydrophilic polymers, these gels (CrysDoS gels) exhibit much higher stretchability than typical hydrogels, breaking the elasticity-toughness trade-off. [3]

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Chloe Shilling (Durham University) - Kinetic Studies of the Cationic Ring Opening Polymerisations of a variety of Poly(oxazoline)s

Oxazolines are a promising alternative to PEG based systems which are used in a lot of applications including formulated consumer products and medicines. Fundamental studies on the synthesis of poly(oxazoline)s with an aim to develop chiral oxazoline, extended oxazolines and bisoxazolines to form novel polymers are being conducted. The poster will describe the kinetic profiles determined so far including investigations into electronic and positional effects. As well as intent for future studies into more complex and chiral oxazolines which could exhibit interesting peptidomimetic secondary structures.

Co-authors: Dr Clare S Mahon, Dr William D G Brittain

Harvey Smart (Durham University) - Synthesis and Analysis of Copper-Loaded Micelles to Address Antimicrobial Resistance

The use of copper complexes in medicine is highly desirable owing to their high stability constants and unique redox chemistry. Previous studies have used copper salts and complexes as adjuvants to address the growing threat of antimicrobial resistance.[1]

Ionophores such as copper pyrithione complexes 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. These enzymes are increasing in prominence worldwide contributing to multi-drug resistance in bacteria. Previous antibiotic synergy studies have shown success using substituted copper pyrithiones particularly against Gram-positive bacteria. However, key issues remain with regards to aqueous solubility and bacterial uptake of these metallodrugs limiting their applicability in medicine.

This project aims to address these issues by modification of the ionophore ligands to increase selectivity and bioactivity, and by the formation of micellar assemblies loaded with the metallodrug. Diblock copolymers have been synthesised from polyethylene glycol and polycaprolactone (PEG-PCL) and self-assembled around the active copper complexes. Furthermore, the copper complexes have been modified directly to produce copper pyrithione - polymer pro-drugs to further help drug loading of the hydrophobic complexes. This has been performed using copper complexes modified with an alcohol group to act as an initiator for the ring opening polymerisation of cyclic esters (Lactide, ε-Caprolactone, and δ-Valerolactone). Micelle formation is characterised by dynamic light scattering, and biological assays will be carried out to assess bioactivity.

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Supreeth Sundar[1] (University of Edinburgh) - Exploring Multiscale Foam Dynamics: Coarsening and Adhesive Forces at Bubble Contacts of Liquid Foams

This study evaluated how aging affected the adhesive, rheological, and mechanical characteristics of liquid foams. Liquid foams are complex materials characterized by a dispersed gas phase within a continuous liquid, stabilized by surfactants. The stability of such foams is influenced by their structural rearrangements over time, particularly through coarsening. Gillette® shaving foam and foam produced by doing a series of ejection/injection cycles of sodium dodecyl sulfate solution through syringe (with stainless steel needle 14G) were used [1]. The Anton-Paar rheometer was used for rheological studies, and an adhesion tensiometer was used to measure the adhesive force curves between foam bubbles. The preliminary results of this study found that (i) at moderate angular frequencies above 5rad/s and below the instrumental limit of 100rad/s the shear moduli agree to the theoretical equations of non-affine bubble motion [2] and the loss modulus follows the scaling law of 0.5. (ii) with aging the elastic modulus shows a clear decreasing trend whereas, the loss modulus initially increases and then decreases which can be interpreted as stages of structural rearrangement and stabilization within the foam. (iii) The adhesive force curves exhibit a soft, sublinear response to small displacements. Aged foams seem to show a smaller elastic scaling in the force curves, correlating with the observed decrease in G' over time, which indicates weakening inter-bubble connections.

This work sheds light on the dynamic interplay between interfacial forces, viscoelastic properties, and foam coarsening. These results encourage a more multiscale comprehension of foam dynamics, which is necessary for the design and development of more stable and sustainable foam-based products.

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