



# ISMC 2025

**9<sup>th</sup> International  
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A photograph of a tall, cylindrical stone lighthouse situated on a rocky island. The lighthouse has a spiral staircase on its exterior and a lantern room at the top. The scene is captured during sunset or sunrise, with a warm orange and yellow sky and a calm sea. In the foreground, there is a small pool of water that reflects the lighthouse and the sky. The background shows distant mountains and a small town on the island.

**Abstract Book**  
**Poster Session 2**



# POSTER SESSION 2

( Wednesday 01/10 - Thursday 02/10)



# F. Fluid Dynamics and Rheology



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# Athermal hard-sphere dense suspensions under general periodic shearing: can the loss tangent detect yielding?

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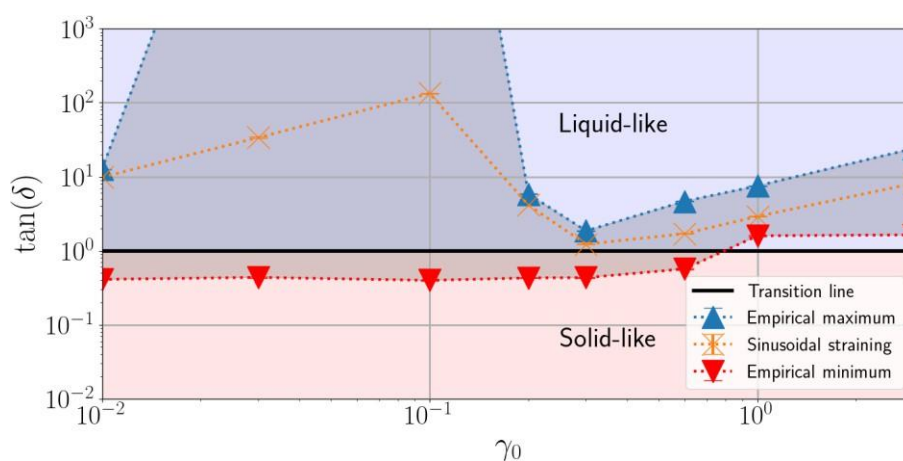
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Viscoelastic materials exhibit both liquid and solid characteristics simultaneously. This broad category includes cement, laboratory polymer mixtures, ketchup, and toothpaste, bridging the gap between conventional solids and liquids. Oscillatory shear (OS) rheology is usually employed to analyze the properties of these materials. This technique measures the storage modulus (elastic response) and loss modulus (viscous response) [1] to provide insights into their solid-like and liquid-like behaviors. For categorizing viscoelastic materials into either solid-like and liquid-like the loss-to-storage ratio, known as the loss tangent, is commonly used.

This work explores the viscoelastic properties of athermal hard-sphere dense suspensions obtained from particle dynamics simulations using general periodic straining protocols beyond sinusoidal via generalized storage and loss moduli. We find that, for a given system trajectory (i.e., where the particles follow the exact paths), one can obtain both a liquid-like and solid-like loss-tangent signal by changing the strain protocol.

We find a large variability of the storage modulus value compared to the loss modulus for our hard-sphere suspensions. This raises the question: how well does the loss tangent actually define a fluid-like to solid-like transition?

**Keywords:** loss tangent, yielding, athermal dense hard-sphere suspension, rheology, oscillatory rheology, viscoelasticity



**Figure 1.** Loss tangent,  $\tan(\delta)$  vs strain amplitude,  $\gamma_0$ .

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## Existence of a lubrication layer piloting the wall slip of dense, polymer microgel suspensions

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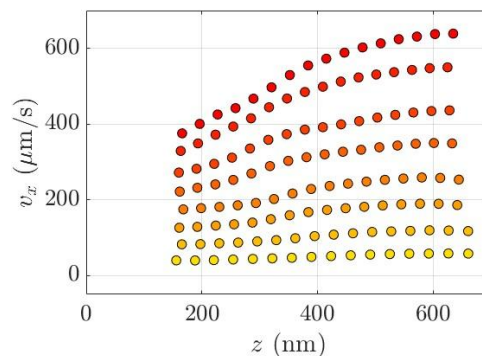
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Microgel suspensions are jammed assemblies of soft, polymeric and colloidal-scale globules. Rheologically, they behave as yield-stress fluids [1]: at low stresses,  $\sigma$ , they are mainly elastic and only flow beyond the yield stress,  $\sigma_Y$ . Moreover, the flow of such materials is highly nontrivial near a smooth, solid boundary [2]. The boundary condition at the solid-liquid interface, as investigated using microscale-resolved experiments, is typically interpreted as exhibiting slip. This apparent slip is usually ascribed to the presence of a solvent-rich, nanometric depletion layer near the layer, yet to be experimentally observed.

In this work, we study the slip of sodium polyacrylate microgel suspensions flowing along smooth walls, using two complementary techniques. Velocity profiles obtained from  $\mu$ -PIV allows us to deduce the existence of an apparent slip velocity [3]. Meanwhile, using total internal reflection fluorescence microscopy (TIRFM), we are able to quantitatively assess the velocity profiles of the flow, within the first micrometer of the solid-liquid interface [4]. As shown on Figure 1, we observe (i) a low-shear region at large distances, and (ii) a highly sheared, near-surface one. Our interpretation is that of the coexistence of two regions: (i) one with a dense suspension of microgels below the yield stress and thus mainly unsheared, and (ii) another where there is a highly sheared lubricating layer near the wall mainly composed of solvent. These measurements represent a first direct observation of the lubricating layer ( $\sim 100$  nm) in dense polymer microgel suspensions flowing along smooth walls.

**Keywords:** yield-stress fluids, evanescent wave microscopy, wall slip phenomena



**Figure 1.** Velocity profiles of 55-nm-radius colloidal particles in a polyacrylate suspension. Concentration: 2 mg/mL; driving pressures: from 200 to 900 mbar.

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## Exploring the competitive effects of hydrophobicity and electrostatics in determining rheology of dense microgel suspensions

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PNIPAM microgel particles undergo a reversible volume phase transition at a volume phase transition temperature, VPTT, in aqueous medium [1]. Dense PNIPAM suspensions transform from a repulsive glass to a colloidal gel phase via a viscoelastic liquid-like phase when temperature is increased across the VPTT [2]. Here, we investigate the collective effect of hydrophobicity and electrostatics on the rheological properties of dense aqueous PNIPAM suspensions over a broad temperature range. Keeping the particle concentration fixed, various dissociative and nondissociative additives were added in dense aqueous PNIPAM suspensions to tune inter-particle interactions and, in turn, the viscoelastic properties of the system. FTIR experiments showed that the hydrophobicity of the suspensions increased as the concentrations of dissociative or nondissociative additives were increased in the suspension medium. Additionally, dissociative additives suppressed screened coulombic repulsion between the particles. Dynamic light scattering experiments further showed that enhanced hydrophobicity led to a systematic reduction in particle size and suspension volume fraction with increase in concentration of both dissociative and nondissociative additives. Oscillatory rheology revealed that hydrophobicity-induced reduction in suspension volume fraction determines the viscoelastic properties of the suspension below the VPTT. This suggests that the concentration rather than the nature of the additives governs the rheological response of PNIPAM suspensions below the VPTT. A double-yielding phenomenon was observed above the VPTT in the presence of both dissociative and non-dissociative additives. The yield strain values strongly depended on the nature and concentration of the additive used, highlighting the additional significant role of electrostatic attraction when dissociative additives were incorporated in the suspension medium above the VPTT. We conclude that both hydrophobicity and electrostatic interactions play a pivotal role in determining suspension behaviour under these conditions. We demonstrate, therefore, that the properties of colloidal microgel suspensions can be tuned easily by tuning inter-particle interaction and medium temperature.

**Keywords:** microgels, additives, hydrophobicity, electrostatic interaction, colloidal gelation.

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## Flow-Induced Margination: A Dissipative Particle Dynamics Approach

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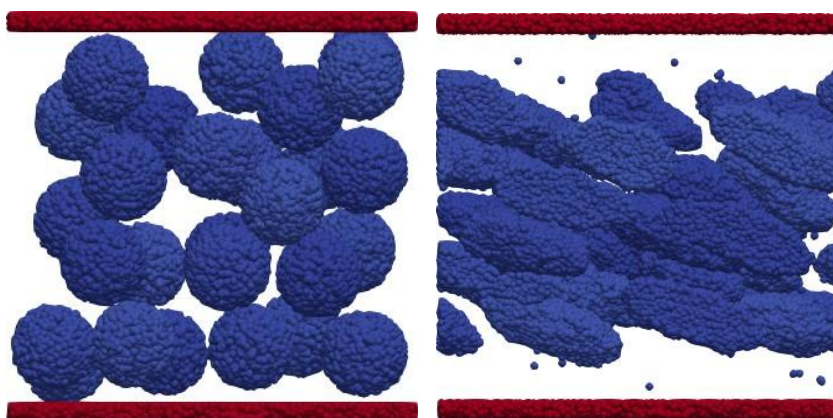
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Margination in blood flow refers to the phenomenon wherein leukocytes and platelets migrate toward vessel walls, while erythrocytes concentrate near the center of the vessel. Previous studies have investigated margination in Couette flow by examining variables such as droplet size, confirming that larger droplets migrate toward the interior while smaller droplets move toward the walls <sup>(1),(2)</sup>. In this investigation, we examine the onset of margination in a Couette flow containing multiple droplets with varying radii using dissipative particle dynamics (DPD) simulations.

Dissipative particle dynamics is frequently employed in soft matter simulations, wherein multiple molecules are aggregated into a single particle. Within the DPD framework, inter-particle forces comprise conservative forces, dissipative forces, and random forces, with numerical calculations executed by solving Newton's equations of motion.

The simulation system consists of a three-dimensional Couette flow configuration, with walls positioned along the y-axis at the upper and lower boundaries, generating shear flow through wall movement in Figure. 1. Simulations were conducted with droplet radius ratios of 1:1.5, 1:2, 1:2.5, and 1:3, with snapshots of the 1:3 ratio case, which exhibited the most pronounced margination effect, presented in Figure 1. The margination tendency became more significant as the radius ratio increased, which qualitatively aligns with previous research findings. These snapshots clearly demonstrate that larger droplets migrate toward the channel interior, where only larger droplets are displayed for clarity. These results confirm that margination can be successfully reproduced using DPD simulation methods.

**Keywords:** Dissipative Particle Dynamics , Margination, Multiphase Flow, Microfluidics



**Figure 1.** Initial position of large droplets (left) and the Snapshot of large droplets at  $\tau = 1000$  (right)

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## Abnormal heat transport in quasi-one-dimensional solutions by molecular simulation

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Recent advances in nanofluidics and nanofabrication present promising opportunities to control thermal properties through nanodevices. For example, molecular dynamics (MD) simulations have shown that monolayer water confined in graphene channels exhibits distinctive thermodynamic properties compared to bulk water [1]. Additionally, coarse-grained molecular simulations have revealed that anomalous heat conduction occurs in elongated nanoscale three-dimensional (3D) fluid systems approaching one-dimensional (1D) behavior [2]. It is well known that heat conduction in low-dimensional systems with conserved total momentum is anomalous and not governed by Fourier's law. However, the conditions under which abnormal heat transport occurs in liquids differ from those in lattice systems [3] and remain poorly understood. Moreover, the impact of polymer additives on anomalous heat transport in liquids is unclear. To address these gaps, we investigated the occurrence of anomalous heat transport in liquids and examined how polymer addition influences heat transport using a coarse-grained hybrid simulation approach that integrates MD with multiparticle collision dynamics. Our results confirm that anomalous heat transport can occur even in liquid-state systems when sufficient anisotropy is introduced. Furthermore, we found that heat transport properties vary with polymer concentration. To gain deeper insight into nanoscale heat transport mechanisms, we also analyzed confined liquids using all-atom MD simulations.

**Keywords:** Abnormal heat transport, Quasi-one-dimensional fluids, Molecular simulation, Self-assembly

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# Dissipative Particle Dynamics Study of Tribological and Flow Properties Induced by the Self-Assembly of Polymer-Grafted Nanoparticles Confined Between Polymer-Brushed Walls

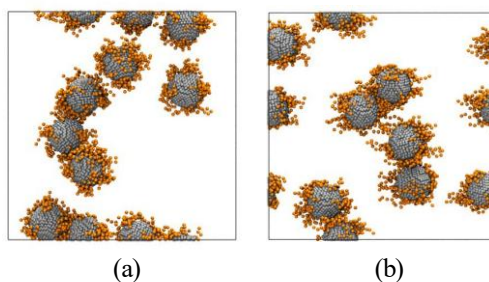
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Contact surfaces grafted with polymers (so-called polymer-brushed walls) have attracted considerable attention due to their excellent lubricating performance [1]. It is also known that the addition of polymer-grafted nanoparticles (PGNPs) to polymer brushes can enhance lubrication through a bearing-like effect and improve mechanical stability [2]. Moreover, the tribological properties of PGNPs confined between polymer-brushed walls are influenced not only by the characteristics of their constituent components but also by their self-assembled structures. Therefore, understanding the relationship between these self-assembled structures and the resulting tribological behavior is crucial for designing materials with tailored properties and functionalities. In this study, dissipative particle dynamics (DPD) simulations were conducted to investigate the effect of PGNP self-assembly on the friction coefficient and shear viscosity of a solution confined between polymer-brushed walls. Two types of polymers and three grafting densities of PGNPs were considered, while shear rates were varied across a wide range. Under good solvent conditions, PGNPs remained well dispersed regardless of graft density, and the coefficient of friction increased as the PGNP graft density decreased. In contrast, under poor solvent conditions, the PGNPs formed clusters whose morphology was sensitive to shear rate—clusters deformed or broke apart depending on the applied shear (Fig. 1). Additionally, the coefficient of friction was found to decrease with increasing graft density under these conditions. The effect of the degree of confinement (i.e., wall separation) was also investigated.

**Keywords:** Polymer-brushed wall, Polymer-grafted nanoparticles, Self-assembly, Molecular simulation



**Figure 1.** Representative snapshots at (a) low and (b) high shear rates for low graft density, respectively.

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## Microchip entrapment using Fluidic gripping

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Accurate and damage-free placement of microchips is critical for high-throughput micro-assembly in applications such as micro LED displays and smartphone components.

In this study, we explore a droplet-assisted alignment method in which water droplets act as soft, reconfigurable interfaces for guiding and positioning 2 mm × 2 mm silicon chips onto receptor substrates. Unlike traditional rigid contact placement, this approach uses surface tension at the water–air interface to temporarily hold and self-align chips, offering a valuable time window for fine adjustments before final bonding. We investigate how key parameters—release velocity, vertical distance, lateral offset, and droplet volume—affect chip landing dynamics, alignment accuracy, and stabilization. Through high-speed imaging and image analysis, we quantify the range of allowable deviations that still yield successful alignment. Our results define the dynamic boundaries of chip placement, helping to identify how much positioning error can be tolerated while maintaining alignment quality.

The study is supported by finite element simulations including fluid–structure interactions. This droplet-mediated technique, with its increased tolerance and extended self-correction window, enables faster machine speeds without sacrificing accuracy and offers a high-throughput alternative for microchip packaging in next-generation electronic devices.

**Keywords:** Droplet-assisted alignment, Microchip entrapment, Surface tension, High-speed imaging, Micro-assembly

## Tuning the rheology of cementitious suspensions with ultrasound

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Controlling the rheological properties of cement-based materials is crucial for a successful application in construction [1]. Currently, the most common method to tailor the rheological behavior of concrete is by adding chemical additives (superplasticizers, viscosity modifying agents) [1]. As an alternative – or complement – to chemical products, this work aims to analyze how applying power ultrasound (PUS) as an external stimulus can help tailoring the fresh state characteristics of cementitious systems. PUS has been used to introduce high energy vibrations and bubble cavitation into several types of suspensions, affecting particle interactions [2]. The use of external stimuli to fine-tune the workability of concrete is a promising area of study, but not yet widely applied in the construction industry [3].

For this purpose, two types of pastes are analyzed: (i) a non-reactive mixture of limestone filler and water, simulating only the physical characteristics of a cement suspension, without the influence of hydration reactions; (ii) a chemically reactive mixture of Portland cement and water. The impact of PUS applied through a sonotrode working at a frequency of 20 kHz and with a power up to 700 W is assessed on both pastes, with varying paste concentration, ultrasound power and duration. Rheological properties such as the static and dynamic yield stresses, the apparent viscosity, the elastic modulus, and the thixotropy are measured using a rotational rheometer (AntonPaar MCR 302) and compared with samples that have not been exposed to PUS. Potential effects of sonication on the temperature of the samples are assessed and controlled when necessary.

From the present study, it is expected that relevant information will be obtained on the action of ultrasound waves on highly concentrated granular suspensions, considering both physical and chemical phenomena (for reactive materials). Also, it is presumed that our results will allow us to identify industrial and construction applications for which the use of PUS could be useful in terms of controlling rheological properties.

**Keywords:** Cement. Limestone. Power Ultrasound. Rheology. Granular Suspensions.

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## Inferring Microstructural Characteristics from the Yielding Behavior of Jammed Suspensions

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In recent years, significant progress has been made in understanding the dynamics of jammed soft colloidal particles, which are prevalent in both natural and industrial applications. To gain deeper insight into yield stress, it is crucial to establish a link between macroscopic mechanical response and local microstructure. In this work we build-up on earlier developments that classifies the yielding of jammed soft particle suspensions based on their interactions (pair potential and faceting-osmotic deswelling-interpenetration) and assess the behavior of model ultrasoft and industrial microgels.

We use well-characterized acrylic microgels with different low degree of crosslinking (ultrasoft particles) and Carbopol, a widely used industrial material, serves as a prime example, yet its microstructure remains largely unresolved. We apply a methodology that leverages the rheological response of structurally well-characterized soft materials in the jamming regime. By identifying characteristic rheological patterns, we correlate their behavior with internal microstructural properties.

Our results are based on well-defined preshear protocols, extend the mapping of microstructure-to-yielding to the case of ultrasoft particles, where deswelling remains a key mechanism of particle arrangement in the jamming regime. They also show that Carbopol despite its complexity and structural heterogeneity, can be effectively considered as a predominantly repulsive microgel suspension.

**Keywords:** yielding, Carbopol, ultrasoft microgels, internal microstructure





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## Pressure, concentration and temperature dependent dynamical investigation of relaxations associated with hydrogen bonding in 1-propanol

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Understanding the dynamics of hydrogen bonds is essential because of their prevalent presence in nature and crucial role in the continual development of technology. Water is the most important hydrogenbonded liquid, of course, but because of its extremely peculiar behavior and challenges with supercooling, exploring it can be challenging. In other hydrogen bonded systems, e.g., in poly-alcohol and biomolecules the dynamics of the hydrogen bonds merge with other dynamics. Mono-hydroxy alcohols have proven to be an interesting case for the study of hydrogen bonds, because the dynamics connected to the hydrogen bonds appears well separated in these systems. The mono-hydroxy alcohols have been studied extensively over the last decades due to their interesting relaxation pattern. Specifically, by dielectric spectroscopy it has been demonstrated that the hydrogen bonds of the monohydroxy alcohols give rise to a dominant relaxation process, the so-called Debye process, which is slower than the  $\alpha$ -relaxation[1-3]. In the past years there is evidence building up that the relaxation of poly-alcohols can in fact also be separated into a Debye like process and an  $\alpha$ -relaxation[4], though the processes are more merged in the case of poly-alcohols compared to mono alcohols. In this work, we plan to better comprehend the dynamical relaxations associated with hydrogen bonds employing quasi- and inelastic neutron scattering under elevated pressure for the case of mono-alcohol 1-propanol in liquid state and above the glass transition. High pressure up to 3Kbar slows the relaxation by two orders of magnitude, and our primary results reveal that the shift in different relaxations is not linear, which further leads to the possibility of separation of individual slower processes. We are also trying to understand if these slower relaxations respond to an increase in H-bond concentration. The concentration of the hydrogen bond is increased by adding the poly-alcohol glycerol to the 1-propanol. It has been observed in our preliminary experiments that the addition of glycerol yields a stronger signal in the slowest part of the signal. We study 1-propanol and its mixture with glycerol in both protonated and partially deuterated samples, where the dynamics of the OH-groups are invisible to the neutrons. The deuteration strongly suppresses the slow part of the signal, which clearly demonstrates that this slow part of the dynamics is due to the hydrogen bonds.

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## Shear thickening in golfball particle suspensions

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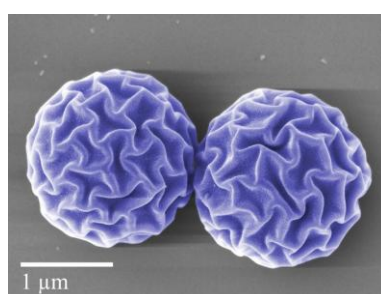
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Dense colloidal suspensions are ubiquitous in nature and industrial applications. Such suspensions display shear thickening when they are subjected to high shear rates/stresses. During this thickening process, the suspension's viscosity abruptly increases, and the material may even become solid under flow, in the most extreme example of thickening called shear jamming. This transition occurs due to particles making frictional contacts and thus creating force chains in the suspension [1,2]. The surface roughness of particles has been shown to strongly influence frictional contacts and therefore lends itself as a tool to tune shear thickening in suspensions [3-5].

Here, as opposed to previous studies on particles with convex asperities, so called raspberry particles, we study the thickening effects of dense suspensions of golfball particles, which offer rough surfaces with concave topography. We quantify the maximum packing fraction for golfball particles with various degrees of buckling and find a strong decrease in the maximum packing fraction for highly buckled golfballs, reflecting their surface roughness. We then characterize the shear thickening properties of various particle types via shear rheology measurements. We find that the suspensions behave similarly to smooth particle suspensions, yet presenting the same rheology at much lower solid loading. This is in stark contrast to the rheological properties of raspberry particles. Intriguing rheological response is finally obtained by mixing golfballs with raspberries due to a lock-and-key mechanism between the two particle species. We clearly find that the surface roughness alone cannot explain our experimental data and that transition from convex to concave surfaces with similar roughness is non-monotonic in its jamming properties. Therefore, the interplay between convex and concave surfaces leads to non-trivial tribological and rheological effects in particle suspension, which we aim to investigate in the near future.

**Keywords:** Rheology, Roughness, Tribology



**Figure 1.** False-colored SEM image of rough golfball particles.

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## Dynamics and self-organization of lipid domains in pure DPPC monolayers

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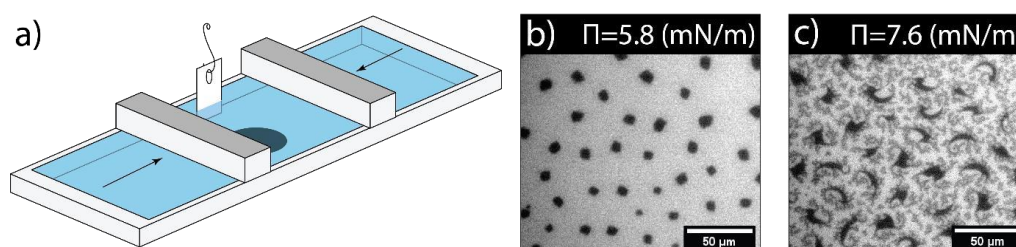
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Lipid monolayers perform essential protective and structural functions in several biological contexts. In the respiratory system, the alveolar surface is lined with a pulmonary surfactant monolayer, which prevents the lungs from collapsing during breathing. This monolayer is primarily a mixture of neutral lipids and proteins, as well as phospholipids of which DPPC is the major component [1]. Understanding the micro and macroscopic behavior of pure DPPC monolayers, therefore, holds considerable physiological relevance. In this work, we study the self-organization of DPPC lipid domains at the liquid-air interface, as a minimal model for biointerfaces. Using a Langmuir-Blodgett trough coupled to an in-house optical microscopy setup, we vary the surface pressure while visualizing the lipid behavior thanks to the presence of a fluorescent lipid (TR-PE). The DPPC monolayer undergoes phase transitions from gas to liquid to solid with increasing surface pressure, displaying a coexistence region where solid DPPC domains form within the liquid phase [2]. We analyze the self-organization and dynamics of these lipid domains by characterizing their size, separation and area fraction while also measuring local order parameters, trajectories and domain spatial correlation as a function of surface pressure. Our findings suggest the presence of correlated motion in domain neighborhoods with increasing surface pressure. These observations will allow us to understand the monolayer's fluidity properties at a fundamental level, providing a basis for scaling up the system with the addition of cholesterol or micron-sized particles as a model for micropollutants.

**Keywords:** Lipid, monolayer, interface.



**Figure 1.** a) Diagram of the Langmuir-Blodgett trough. b-c) Fluorescence microscopy images of the monolayer, showing the solid domains (dark regions) and their shapes for different values of the surface pressure.

**Acknowledgements:** The authors would like to thank the ANR for its support (Appollo-ANR-23CE06-0035)

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## Visualising energy dissipation on superhydrophobic surfaces

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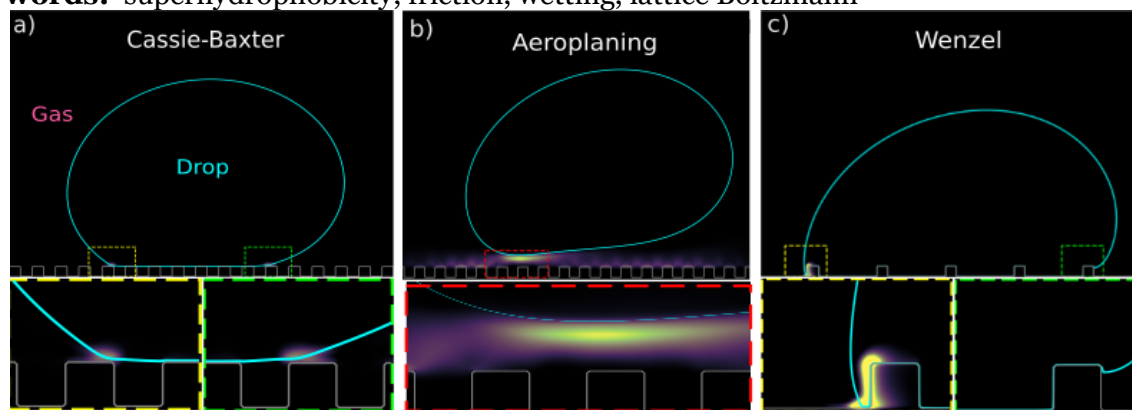
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Inspired by the lotus leaf, superhydrophobic surfaces are structured surfaces that have attracted significant attention for their anti-icing, anti-biofouling, and self-cleaning properties. Most of these useful properties arise because liquid drops exhibit remarkably low friction on these surfaces, reaching velocities as high as several cm/s. The velocity that the drop can reach depends on the amount of direct contact between the drop and the structured surface. Drops can assume three distinct states on superhydrophobic surfaces, as shown in Fig. 1. In the Cassie state, the drop sits on top of the surface protrusions making only partial contact with the solid. In the Wenzel state, the drop penetrates the surface structures, making full contact. In the recently discovered [1,2] ‘aeroplaning state’, the droplet partially or completely lifts off the surface, resulting in minimal solid/liquid contact. Despite these observations, how energy is dissipated in these systems, which is important for understanding friction, remains poorly understood.

To address this, we use lattice Boltzmann simulations to visualise and quantify how energy is dissipated when drops move in the three different states. We find that in the Cassie state, energy is dissipated primarily within the droplet and is dominated by pinning and depinning events at the droplet's leading and trailing edges (Fig. 1a). In contrast, for the aeroplaning state, energy dissipation is concentrated in the air layer beneath the droplet and is highest in the bottleneck region at its rear (Fig. 1b). In the Wenzel state, energy dissipation is highest when the trailing edge moves from the base of a pillar to the top of the pillar (Fig. 1c).

These findings provide a comprehensive understanding of how the amount of solid/liquid contact influences how energy is dissipated on structured surfaces.

**Keywords:** superhydrophobicity, friction, wetting, lattice Boltzmann



**Figure 1.** Heatmaps of viscous dissipation for a droplet (cyan contour) moving over a structured surface (grey).

**Acknowledgements:** The authors would like to thank EPSRC for funding AA through SOFI<sup>2</sup> CDT, AN with fellowship EP/X028410/2, and HK with fellowship EP/VO34154/2

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## Deposition dynamics in asymmetric coffee rings

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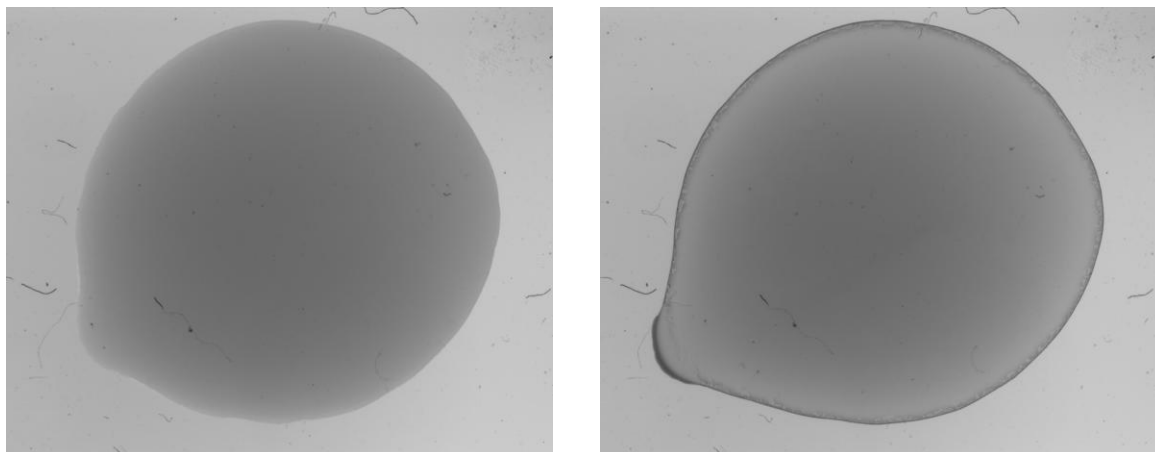
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The coffee ring effect is a ubiquitous phenomenon observed in evaporating droplets containing suspended particles, commonly witnessed in everyday life through stains left by dried beverages such as coffee, tea, or wine. This effect manifests as a darkened peripheral ring, formed due to the accumulation of solute particles at the droplet's edge during evaporation. The underlying mechanism is driven by capillary flow: as evaporation occurs more rapidly at the droplet's edge—where the contact line remains pinned—liquid from the interior flows outward to replenish the loss, transporting suspended particles toward the periphery [1]. However, droplets rarely stay axially symmetric, and irregularities in the curvature of the contact line induce asymmetric accumulation of the material at the rim.

To understand the relationship between the curvature and ring formation dynamics, we use optical microscopy to study the temporal changes of optical density of drying droplets and quantify the mass density distribution throughout the evaporation process. We examine the associated bulk flow. Using coffee as working fluid, we reproduce the original effect known from culinary fluid dynamics [2]. In addition, we vary coffee powder grind size to alter the solute particle size distribution but retaining a realistic variability.

The curvature of the initial droplet determines both the shape and size of the coffee ring. We study how variations of the key parameters, such as initial solute concentration and droplet volume, affect the dynamics of ring formation.

**Keywords:** Coffee ring effect, evaporation, sediment transport, deposition, particle-laden flows



**Figure 1.** Optical microscopy images of an asymmetric coffee droplet of ca. 1 cm in diameter, freshly spilt (left) and fully dried (right). Clear differences in the rim thickness are visible at locations of increased curvature.

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## Experimental Study of Peristaltic Flow in Annular Geometries with Deformable Boundaries

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Peristaltic flow in elastic annular geometries, induced by propagating waves along elastic boundaries, is a fundamental flow mechanism with significant implications for physiological systems. For example, this mechanism, generated by cardiac pulsations, was hypothesised to drive cerebrospinal fluid flow inside the brain [1]. Experimental studies on peristaltic flow in these geometries remain limited, highlighting the need for further investigation.

We present a novel experimental approach using refractive index-matched elastic materials to study peristaltic flow in elastic annular domains. Our setup, presented in Fig. 1, consists of an elastic inner tube and a transparent PDMS outer boundary which can be fabricated with varying properties, forming an annular channel. This design provides the optical clarity essential for detailed flow visualization while maintaining and controlling geometric and material properties. Using pressure-controlled pulsation of the inner tube, we generate propagating waves that induce fluid transport along the annular space. The flow is evaluated and quantified via high-resolution particle tracking experiments and the elastic tube behavior is measured using image analysis.

Our findings reveal that net peristaltic flow is induced in the direction of the propagating wave, with velocity increasing with pulsation pressure. We also found that volumetric flow rates increase nonlinearly with pulsation pressure, following a quadratic relationship consistent with the analytical expression for the time-averaged flow rate developed by Wang and Olbricht [2]. These results provide new empirical data that complement recent theoretical and numerical studies in this field.

This work introduces an experimental framework for analyzing peristaltic flow in complex annular geometries with elastic boundaries, addressing fundamental questions about how material properties and pulse characteristics influence the resulting flow.

**Keywords:** peristaltic flow, fluid-structure interaction, deformable boundaries



**Figure 1.** Experimental setup (left) and representative frame from an experiment (right).

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## Rheomicroscopy of Hydrogels across the Yielding

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Hydrogels are soft, water-rich polymer networks with wide applications in biomedicine and soft robotics. A key performance threshold in these materials is yielding—the point where the gel stops behaving like an elastic solid and begins to flow. (1) While bulk rheology identifies when this transition occurs, it doesn't reveal the microscopic changes that drive it.

In this work, I combine strain-controlled rheology—including amplitude sweeps, frequency sweeps, and LAOS—with real-time microscopy techniques to observe structural evolution during deformation. (2, 3) I use rheomicroscopy, Differential Dynamic Microscopy (DDM), and Echo-based microrheology (ECHES) to track how the gel's internal structure changes during deformation, including small shifts, local breakages, and uneven movements.

My focus is on mechanical training—the process of applying repeated sub-yield strain to adapt and reinforce the gel's mechanical response without causing damage. I also vary the crosslinking density to understand how network architecture influences both the onset of yielding and the gel's ability to encode mechanical memory.

This poster presents preliminary results from experiments conducted using both commercial and custom-built rheometers, revealing how hydrogels respond under different mechanical protocols. By connecting bulk mechanical signatures with microscopic dynamics, this study aims to develop a multi-scale understanding of how hydrogels yield, adapt, and potentially “learn” from stress.

These insights contribute to the goals of the TRAINGEL project, which seeks to engineer hydrogels with programmable, robust mechanical properties for next-generation biomedical and soft-material applications.

**Keywords:** Hydrogels, Rheomicroscopy, Microstructure, Soft materials

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## Viscoelasticity and extensional rheology of polystyrene based vitrimers

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A formidable challenge in soft matter is to develop crosslinked materials that combine the reprocessing capabilities typical of thermoplastics with the shape stability and mechanical strength of conventional thermosets. Most approaches aim to create a crosslinked network using dynamic covalent bonds, which can reversibly form and break in response to changes in thermodynamic conditions. Materials containing these dynamic covalent bonds are referred to as Covalent Adaptable Networks (CANs). A specific subset of CANs, known as vitrimers, was introduced by Leibler and colleagues in 2011. Vitrimers exhibit two key characteristics: they maintain stable network connectivity across a range of temperatures and can relieve mechanical stresses through bond exchange reactions.

In this work, we present preliminary results on the extensional rheology of polystyrene- based vitrimer systems, where dynamic exchange reactions are facilitated by dioxaborolane metathesis. We show how crosslink density and dynamic bond exchange influence the flow and deformation behavior under both linear and nonlinear deformations, which are particularly relevant for processing operations. In particular, a systematic investigation of the uniaxial extensional response of vitrimer systems is presented, detailing how the presence of dynamic crosslinkers affects strain hardening behavior.

These insights contribute to a deeper understanding of the fundamental rheological behavior of polystyrene-based vitrimers and their potential for use in advanced material design.

**Keywords:** vitrimers, rheology, uniaxial extension

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## Extension and Scission of polymers under high shear rates in microfluidic chips

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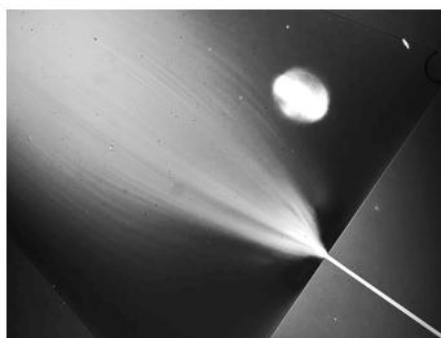
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Microfluidic devices are ideally suited for the study of complex fluids undergoing large deformation rates in the absence of inertial complications [1]. Previous studies involving conventional narrow-width microfluidic channels faced challenges accurately measuring the flow-induced deformation of long-chain polymers, due to significant measurement uncertainties and limited precision [2]. In this research, we introduced a microfluidic chip fabricated specifically to provide accurate measurements of flow-induced birefringence in polymer solutions by polarized optical microscopy. As shown in Figure 1, the polymer solution (100K PEO, 1 wt % in water) was pumped into the microfluidic chip at a flow rate of 10 ml/h. In the central microchannel with a height of 20  $\mu\text{m}$  and a width of 20  $\mu\text{m}$ , the long-chain polymer molecules became oriented along a specific direction due to the flow-induced extension, forming flow-induced birefringence.

Another comparative viscosity chip, combined with high-speed micro-particle image velocimetry ( $\mu\text{PIV}$ ), was used to precisely measure the viscosity changes under high shear conditions. Furthermore, Gel permeation chromatography (GPC) was employed to determine molecular weight distributions accurately. The sample, after the treatment in Figure 1, exhibited a clear decrease in molecular weight, with the number-average molecular weight ( $M_n$ ) dropping to 45.14K. This indicates that the PEO sample underwent chain scission under high shear flow conditions. Moreover, the pronounced reduction in molecular weight demonstrates that the high shear flow is particularly effective at causing scission of longer polymer chains, confirming that high shear flow is more effective in breaking long-chain polymers. This comprehensive approach offers enhanced accuracy in analyzing the viscosity behavior of polymers under flow conditions. Such an approach provides valuable insights into polymer rheology, drug delivery systems, and industrial production processes.

**Keywords:** Polymer Scission, Microfluidic, GPC, Flow-birefringence



**Figure 1.** Birefringence phenomenon observed under polarized optical microscopy

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## Kneading as an efficient mixing method to enhance processability of graphite anode slurries

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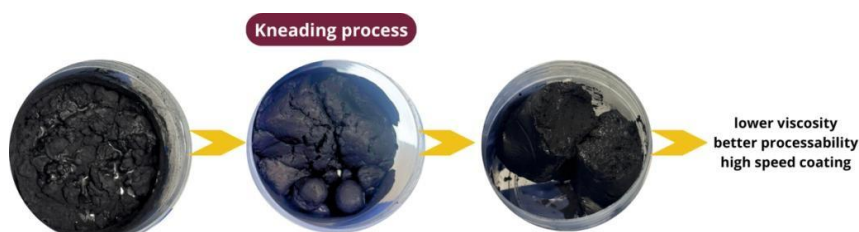
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Graphite anode slurries for lithium-ion batteries require precise control of rheological properties to ensure optimal electrode performance. Traditional sequential mixing: CMC solution, carbon black, graphite and SBR often yields high-viscosity slurries with gel-like behavior, requiring long time mixing. [1] This study introduces kneading - a process adapted from food-industry dough preparation where solid components and binders are mixed cohesively at high shear to form an elastic, "dough-like" slurry. [2] The kneading process was systematically contrasted with traditional method, examining how processing parameters govern the rheology and microstructure of nonNewtonian slurries.

Rheological characterization such as flow curves and oscillatory tests reveals that kneading reduces viscosity 1.6-1.8 times compared to traditional mixing, preventing excessive gelation and enhancing fluidity for coating. At the critical "kneading point," slurries achieve uniform binder distribution and lower yield stress. The critical kneading point was identified via penetration tests using a tensile meter, which correlates with optimal slurry plasticity and uniform binder distribution. SEM analysis further confirms kneading's role in homogenizing microstructure, eliminating agglomerates prevalent in traditional slurries.

Our findings demonstrate kneading's advantages in producing low-viscosity, high-solidcontent slurries with scalable electrode fabrication. This shift from sequential mixing to dough-based processing offers more effective dispersion, which can result in overall better electrode performance.

**Keywords:** lithium-ion battery, kneading, rheology, slurry processing



**Figure 1.** Kneading process and its advantages.

**Acknowledgements:** This project is funded from the European Union's Horizon Europe Framework Programme (HORIZON) under the Marie Skłodowska-Curie Grant Agreement (GA) N°: 101120301.

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## Monovalent and Divalent Cation Transport in PEO Electrolytes: Role of Molecular Weight and Cation Chemistry

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As the demand for sustainable energy storage intensifies, alternative chemistries beyond lithium-ion are gaining momentum—most notably, sodium-ion batteries, which offer advantages in cost, abundance, and safety. A key challenge to their development lies in engineering efficient solid polymer electrolytes that combine high ionic conductivity with robust mechanical properties. In this study, we investigate how cation identity and polymer architecture collectively influence ion transport and mechanical behavior in poly(ethylene oxide) (PEO)-based electrolytes. Two PEO systems—high molecular weight ( $M_w = 100$  kg/mol) and low molecular weight ( $M_w = 0.35$  kg/mol)—were blended with a series of monovalent ( $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ) and divalent ( $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ) TFSI salts across a range of salt-to-ether oxygen ratios. Our results reveal distinct ion transport mechanisms that depend strongly on PEO molecular weight: in high- $M_w$  PEO, ion hopping favors smaller, more strongly coordinated cations (e.g.,  $\text{Li}^+$ ), while in low- $M_w$  PEO, segmental diffusion supports enhanced mobility for larger cations like  $\text{Na}^+$  due to weaker coordination and reduced hydrodynamic drag. Notably, NaTFSI in low- $M_w$  PEO achieves room-temperature conductivities approaching  $4 \times 10^{-4}$  S/cm — comparable to state-of-the-art values for solidstate Na-ion conductors.

**Keywords:** cation chemistry, ion transport, PEO electrolytes.

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# I. Interfaces, surfaces, membranes, emulsions



## Development of Superhydrophobic and Antifouling Surfaces Utilizing Polymer Nanocomposites

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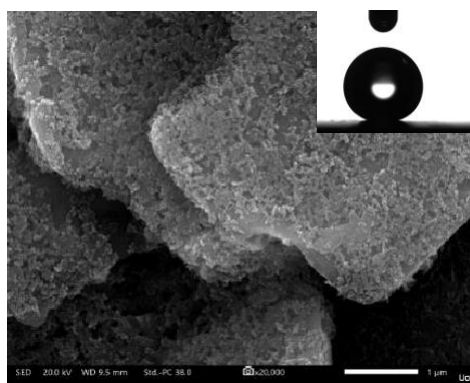
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The development of surfaces exhibiting superhydrophobicity and water repellency, inspired by natural systems such as lotus leaves, has emerged as a field of increasing scientific interest due to its potential applications in self-cleaning, antifouling, and fluid manipulation technologies. In this study, polymer nanocomposite coatings are designed to impart superhydrophobicity and water repellency to surfaces, enhancing their antifouling efficiency. This was achieved by depositing nanohybrid coatings that incorporate a hydrophobic polymer and different additives like  $\text{Al}_2\text{O}_3$  and  $\text{TiO}_2$  nanoparticles or layered materials such as MXene, or even a combination of both. The wetting properties of the coated surfaces were evaluated via contact angle and contact angle hysteresis measurements, the morphology of the coated surfaces was examined using Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM), while the surface chemical composition was determined via Energy Dispersive Spectroscopy (EDS). The nanohybrid composition was optimized to achieve the desired wetting properties. For the optimized coating, a superhydrophobic ( $\text{CA} > 150^\circ$ ) and water repellent (hysteresis  $< 5^\circ$ ) surface was obtained. Moreover, the stability of the coated surfaces over time, under increased temperature and upon chemical treatment as well as under friction was investigated.

**Keywords** Superhydrophobic surfaces, Water repellency, Polymer nanocomposites, Nanohybrid coatings



**Figure 1:** SEM image and corresponding contact angle measurement of nanocomposite coatings with MXene- $\text{Al}_2\text{O}_3$

**Acknowledgements:** This research has been partially financed by the EU Horizon Europe Programme (project STOP, Grant Agreement 101057961).



## **No time for surface charge: how bulk conductivity can hide charge patterns from KPFM**

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Soft materials are used ubiquitously in experimental fields ranging from microfluidics to granular matter to metamaterials. In many cases, these experiments are sensitive to stray electric fields caused by surface charge. Soft materials readily gain and retain surface charge through contact electrification (CE), due their high elastic compliance. Even so, the mechanism of CE, especially with disordered soft materials, remains poorly understood [1, 2].

A powerful tool for studying CE is Kelvin probe force microscopy (KPFM), where electrical signals from an AFM tip allow one to spatially map a voltage above a surface that is caused by the presence of charge [3]. Among the most influential results obtained with KPFM are observations of surface charge heterogeneity, i.e. mosaic-like patterns of +/- polarity after CE [4]. For such experiments, we use PDMS, due to its ability to create conformal contacts. In trying to reproduce such results, we instead observe signatures of spatially uniform surface potential that displays prominent temporal decay over a few minutes [5].

We propose that this is due to the material's bulk conductivity, which lowers the KPFM potential via the movement of non-CE charge carriers in the electric field gradient between the surface and back electrode. Using a simple capacitor model, we attribute the observed decay to bulk conductivity. The timescales of this decay vary across different soft polymer surfaces, aligning qualitatively with their electrical conductivities. Our results call into question the presence/stability of surface charge patterns on certain materials, and highlight the role of bulk conductivity during and after CE.

**Keywords:** Contact electrification, Kelvin probe force microscopy, electrostatic interactions, tribology

**Acknowledgements:** This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 949120).

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## Giant mobility of surface-trapped ionic charges following liquid tribocharging

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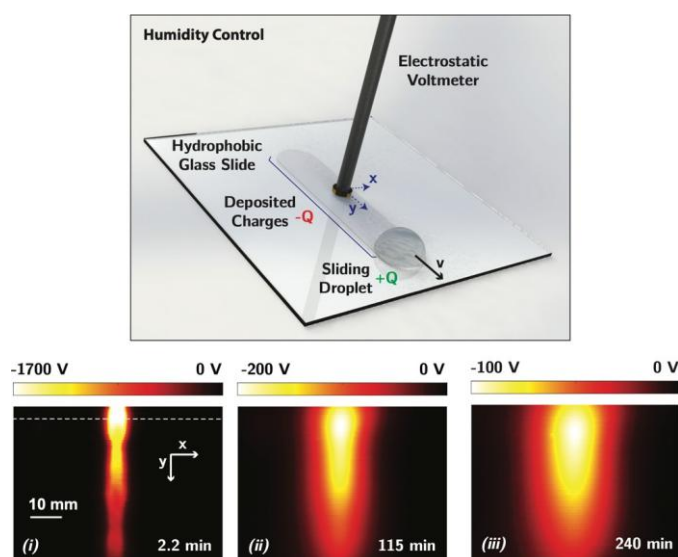
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The sliding motion of aqueous droplets on hydrophobic surfaces leads to charge separation at the trailing edge, with implications from triple-line friction to hydrovoltaic energy generation. Charges deposited on the solid surface have been attributed to stem from ions or electrons ripped off from the liquid drop. However, the dynamics and exact physicochemical nature of these surface-trapped charges remains poorly explored. Here, we take advantage of a scanning-based electrostatic mapping technique, to directly quantify the spatiotemporal dynamics of surface deposited charges in the wake of droplets sliding on hydrophobic surfaces. We confirm the ionic nature of these interfacially trapped charges, and evidence that they undergo very fast bidimensional diffusive transport, gliding with low friction at the solid/gas interface. We rationalize our observations through molecular dynamics simulation of hydrated ions adsorbed on solid surfaces, revealing a peculiar transport mechanism limited by purely interfacial friction of the ionic solvation shell with the solid surface. By uncovering the unexpected dynamics of these *ionic puddles* - a new state of interfacial ionic matter - our findings have general implications for molecular-scale ionic transport and electrified matter at interfaces.

<https://arxiv.org/abs/2503.04987>



**Figure 1.** Schematic of the experimental setup. An aqueous droplet slides on a hydrophobic surface, leading to surface electrification and deposition of negative charges on the solid. The associated 2D surface potential is measured by scanning an electrostatic voltmeter over the surface. Temporal evolution of the associated surface potential, evidencing the surface diffusion of deposited charges.



## Understanding Stress Recovery from Poly (Styrene-block-Butadiene-block-Styrene) Triblock Copolymer

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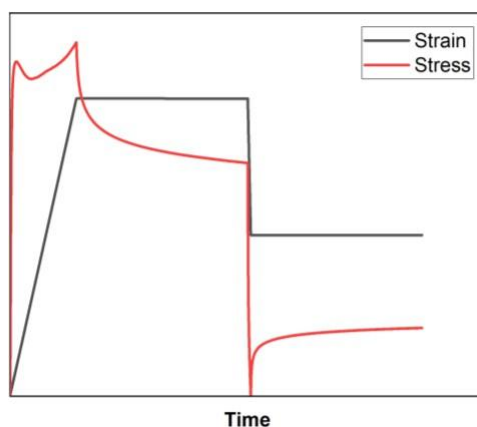
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Styrene based block copolymers exhibit shape memory properties as they demonstrate mechanical and structural recovery after deformation. This study explores the stress recovery behaviour and structural evolution of a poly(styrene–block-butadiene-block-styrene) (SBS) triblock copolymer subjected to strain. By analysing its response to deformation, we aim to uncover the mechanisms responsible for stress relaxation and stress recovery in the polymer.

We perform uniaxial deformation where we stretch the film till a fixed strain and hold it. While the SBS is elastomeric, the stress developed on straining relaxes when the sample is held at a fixed strain. We subsequently decrease the strain till stress in the film becomes zero. Holding the film at that strain results in stress recovery (Fig. 1). We observe stress recovery even for strains lower than yield strain of the polymer. We investigated the recovery behaviour both before and after yield and found that while recovered stress depends on the applied strain across the entire strain regime, it depends on the stress relaxation time only in the pre-yield region. We found that recovered stress increases with strain up to the yield strain, beyond which it decreases.

We utilize small angle X-ray scattering (SAXS) to look at structural changes in the film while deforming to relate the mechanical properties to structural changes in the polymer.



**Figure 1.** Protocol for stress recovery.

**Keywords:** SBS, Tensile Deformation, Stress Recovery, Yield



## Low-dimensional Ionotronics: How Classical Models Reveal New Insights

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Low-dimensional ionotronic systems—electrolytes confined within ordered, conductive nanostructures—exhibit fascinating physics and find a wide range of technological applications, such as capacitive energy storage, desalination, and electroactuation. However, their inherent complexity and the high computational cost of molecular simulations pose significant challenges for theoretical and numerical investigations [1]. In this contribution, we will explore how analytically solvable classical models of statistical physics provide new insights into the behavior of nanostructured ionotronic systems. I will present findings from both lattice [2,3] and off-lattice [4] models, highlighting their relevance to key phenomena such as ion ordering [5], quantum capacitance effects [6], and strategies for optimizing ionotronic device performance [7,8]. Special emphasis will be placed on results that are difficult to obtain through conventional molecular simulations, demonstrating how analytical approaches uniquely advance our understanding of fundamental mechanisms and can guide the design of next-generation ionotronic systems.

**Keywords:** Ionotronic systems; low-dimensional electrodes; capacitive energy storage; nanostructured electrodes; quantum capacitance

**Acknowledgements:** This work was supported by the Polish National Science Centre (NCN) under grants Nos. 2021/40/Q/ST4/00160 and 2020/39/I/ST3/02199.

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## Enzymes at liquid interfaces: linking surface & catalytic activity with foam stability

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Enzymes, capable of catalyzing the breakdown of specific chemical bonds, play a crucial role in various industrial and biological processes. They are widely used in fields such as biotechnology, pharmaceuticals, and pollutant treatment [1]. However, their activity and stability can be limited in complex environments. Fluid interfaces, such as air-water interfaces, can modify the structure of interfacially active enzymes and consequently their catalytic efficiency [2]. Many interfacially active enzymes are also known to stabilize foams like lipase. Here we will show how surface activity and catalytic activity of the lipase can be related to the foam stability. To achieve this, a multi-scale study of lipase enzymes at interfaces is employed, ranging from the analysis of individual bubbles to study enzyme-interface interactions to the formation of foams to evaluate enzyme stability in structured fluids. First, interfacial tension & dilational rheology measurements will be presented to characterize lipase adsorption dynamics at the interface of a single bubble. Then, different foaming measurements will assess the ability of the enzymes to stabilize aqueous foams. The influence of key parameters like lipase concentration and pH on stability and catalytic efficiency at simple (single bubble) and complex (foam) interfaces will be demonstrated. Techniques such as spectroscopy and confocal imaging provide complementary information on the structure and organization of lipases at interfaces.

This work provides a fundamental understanding of enzyme-interface interactions and their role in structured fluids such as foams. By linking the catalytic and surface activity of enzymes to foam stability, we not only provide new insights into enzyme functioning in confined environments. We also open the way to the development of enzymatic foams for applications.

Keywords: Enzymatic activity, Surface activity, Foam stability, Fluid interfaces.

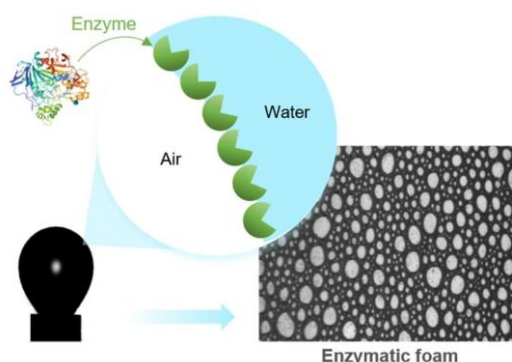


Figure 1. Schematic diagram of the methodology investigating enzyme coated bubbles and foams

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## Surface tension at the critical micelle concentration

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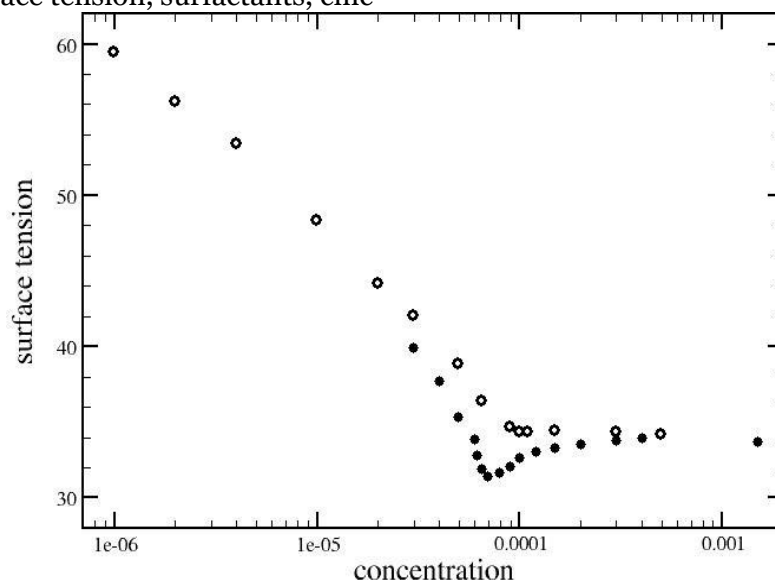
In the 1940's, it was noticed that the surface tension of the interface between a surfactant solution and air, would sometimes exhibit a clear minimum ('dip') when plotted as a function of the surfactant concentration (see the Figure). This seemed in contradiction with the Gibbs adsorption equation which says that a rise in surface tension would indicate **desorption** of the surfactant, which seemed quite unlikely.

A resolution of this problem was first offered by Miles [1] in the suggestion that a tiny amount of impurity must still be present. Indeed it was experimentally verified that rigorous and repeated purification of the surfactant would ultimately lead to the expected monotonous decrease of the surface tension [1]. Furthermore, since then, numerous experiments have been carried out in surfactant mixtures to systematically investigate the magnitude of the 'dip' in surface tension [2].

Mixtures of surfactants and their adsorption to interfaces, have also received a lot of theoretical attention [3]. Theoretical descriptions have been put forward to describe the tension and structure of the interface in the context of sophisticated surface equations of state. Even though the structure and tension at concentrations below the cmc are well-described, it proved difficult to describe the 'dip' in the surface tension in a *quantitative* manner.

In this presentation, a statistical thermodynamical approach is offered leading to an explicit formula for the surface tension of surfactant mixtures as a function of surfactant concentration. The formula is compared to surface tension results for both non-ionic and ionic surfactant systems.

**Keywords:** surface tension, surfactants, cmc



**Figure.** Experimental results for the surface tension as a function of surfactant concentration by Lin et al [2]. Open symbols denote the purified C12E8 surfactant system whereas closed symbols are with 0.1 mol % dodecanol added.

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## Microtribology on Soft Substrates: Sliding and Rolling Friction

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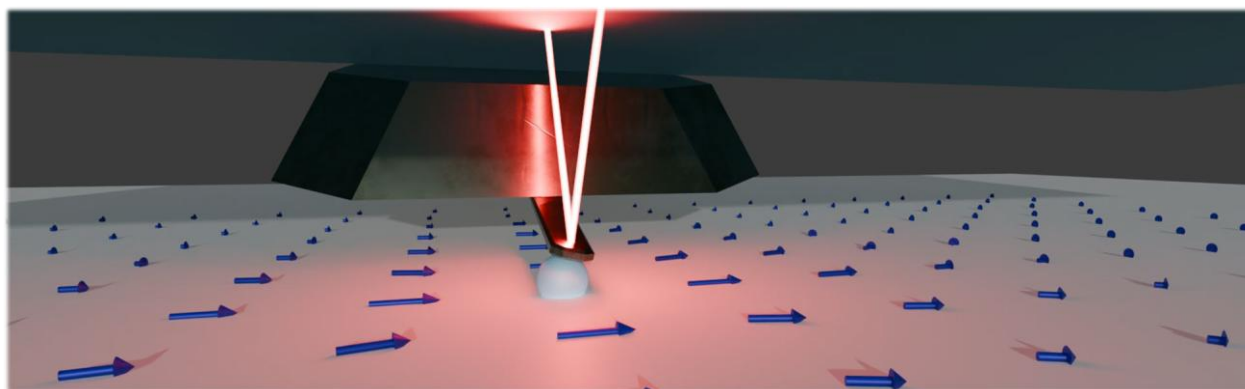
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Lateral force microscopy (LFM) traditionally measures sliding friction by quantifying lateral forces between a fixed probe on a cantilever and a countersurface. Recently, our group developed a novel LFM approach that enables the measurement of rolling friction for free particles. [1] This method combines LFM with fluorescence microscopy, where a fluorescently labelled particle is confined in a microprinted concave holder while rolling or sliding during measurement. This setup allows simultaneous tracking of particle rotation and friction, enabling rolling friction measurements at the microscale.

Building on these advancements, this project focuses on tribological behaviour on compliant adhesive substrates. While sliding friction is well studied [2], rolling friction on soft substrates at the microscale remains largely unexplored. Our research addresses this gap, providing insights relevant to biomedical applications, soft robotics, and wearable electronics.

We begin with sliding friction before advancing to rolling friction. We measure lateral forces between a fixed colloidal probe and nanoparticle-covered polydimethylsiloxane (PDMS), as illustrated in Figure 1. The resulting PDMS deformation is visualised using confocal microscopy and quantified by tracking nanoparticle displacements. We then compare measured friction forces with theoretical calculations derived from nanoparticle displacement data using point force solutions for linearly elastic half-spaces. Evaluating these comparisons across parameters such as substrate stiffness, viscoelastic properties, and the colloidal probe's size, topography, and velocity could yield valuable insights.

**Keywords:** lateral force microscopy, soft tribology, rolling friction, traction force microscopy



**Figure 1.** Illustration of a sliding experiment with a colloidal probe on nanoparticle-covered PDMS. LFM quantifies cantilever torsion, induced by lateral friction, by detecting position shifts of laser reflection (red beam). Substrate deformation is measured by tracking nanoparticles on the surface. The blue arrows represent the displacement field.

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## How mixed-linkers transform fluid intrusion in MOFs

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Metal-organic frameworks (MOFs) are porous materials that can be tuned and can exhibit lyophobic behavior, leading to distinct phase transitions such as pseudo-condensation and pseudo-evaporation in confined fluids [1, 2]. These transitions are strongly influenced by the material's structural and chemical characteristics. A stochastic model was employed to investigate the impact of linker-level heterogeneity on the macroscopic behavior of a mixed-linker ZIF-7-8 system, in which methylimidazolate (mIm) linkers are partially replaced by benzimidazolate (bIm) linkers (1-30%). The model captures the probabilistic nature of fluid intrusion and extrusion at the cage level under an applied external pressure, providing insights into the influence of bIm linkers on hysteresis.

The results indicated that even small concentrations of bIm (as low as 1%) significantly affected intrusion and extrusion pressures. The presence of bIm disrupted hydrogen bonding across 6-membered ring apertures in the ZIF-7-8 structure, increasing energy barriers for water intrusion and destabilizing the confined fluid phase. Hence, hysteresis decreased with increasing bIm concentration, reducing the energy dissipation associated with intrusion-extrusion cycles. These local modifications in the framework altered the global response, impeding intrusion and facilitating the extrusion by weakening fluid-cage interactions, reshaping the energy landscape and influencing adjacent cages.

Consistent agreement with experimental observations showed that minor bIm concentrations can systematically tune hysteresis and energy absorption. These findings provided a basis for designing porous materials with tailored pressure sensitivity and energy dissipation, enabling applications in energy storage, pressure-sensitive devices, and vibrational damping for shock mitigation.

**Keywords:** MOFs, intrusion, stochastic modeling, energy dissipation

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## The rheological perspective of phase transition in soft solids

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Soap is any molecule formed by the reaction of an alkyl carboxylic acid with a base. The sodium and potassium soap exist as an array of self-assembled structures in water ranging from crystalline solids, and liquid crystals to micellar and monomeric liquids. The pH, temperature, and concentration at which these structures form in water is strongly dependent on the nature of the hydrocarbon chain. For instance, two soaps, sodium stearate (C18) and sodium palmitate (C16), can depict a rich variety of phase structure transitions across phase boundaries as a function of concentration and temperature. We report this work on a single transition from a micellar phase to a solid phase for these two soaps using rheology as a tool. The aqueous dispersion is prepared by dissolving a predetermined amount of soap in deionized water and this system undergoes the liquid-solid transition upon decreasing the temperature. The dependence of dynamic moduli at different temperatures illustrates this transition passing through the critical state followed by a sudden increase in elastic modulus ( $G'$ ) as the temperature decreases. The characteristic feature enveloping the variation of cooling rate and salt concentration renders a rheological understanding as elastic modulus ( $G'$ ) evolves faster than viscous modulus ( $G''$ ) beyond the critical point [2]. This study represents a keen insight into the phase transformation with liquid-like properties to a solid state due to temperature change which many times is reversible in nature. Furthermore, study of the flow of materials, soaps with yield stress typically exhibit yielding behavior, as they behave as a solid upto a certain applied stress and start flowing as a liquid once this stress value is exceeded. This is important for formulations like shaving creams, where a specific consistency is desired for ease of application.

**Keywords:** Phase transition, Dynamic moduli, Critical temperature, Yield stress

**Acknowledgments:** We acknowledge the financial support from the Anusandhan National Research Foundation (ANRF), the Department of Science and Technology (DST), Government of India (GoI).

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## Functionalized octaspherosilicates and cyclosiloxanes as novel emulsifiers

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In recent years, scientists and commercial sector have been actively seeking new emulsifiers to ensure the long-term stability of colloidal systems. Emulsifying agents are crucial for reducing interfacial tension between two immiscible phases promoting droplet formation and preventing coalescence [1]. Modified organosilicon compounds, such as derivatives of silsesquioxanes, have been examined as potential emulsifiers [2,3]. It was demonstrated that bifunctionalized silsesquioxanes exhibited superior emulsifying properties compared to their monofunctional analogues.

The aim of this study was to synthesize and evaluate the emulsifying properties of octaspherosilicates and cyclosiloxanes modified with hydroxybenzophenone and polyethylene glycol (PEG) groups in various molar ratios. These compounds were synthesized in hydrosilylation reaction using Karstedt's catalyst, followed by spectroscopic analyses. The hydrophilic-hydrophobic nature of organosilicons was assessed by contact angle measurements. Afterwards, the emulsions containing functionalized octaspherosilicates or cyclosiloxanes were prepared and their stability was monitored by centrifugation test, multiple light scattering, laser diffraction and optical microscopy. It was proved that the more polyethylene glycol groups attached to either octaspherosilicates or cyclosiloxane core the more stable the emulsion. It was also demonstrated that the key factor influencing the stability of emulsion was the optimal selection of the water to oil phase ratio for each organosilicon compound.

**Keywords:** organosilicon compounds, emulsions, stability studies, multiple light scattering,

**Acknowledgements:** The research was financially supported by The National Centre for Research and Development (Poland), grant number LIDER/5/0036/L-12/20/NCBR/2021.

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## Understanding the Role of Particles in the Interfacial and Bulk Rheology of Pickering-Ramsden Emulsions

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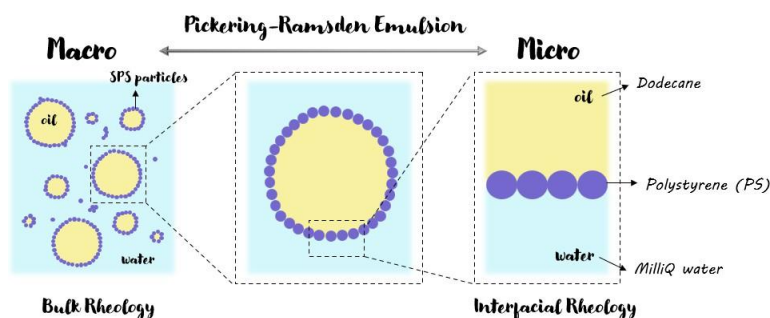
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In today's world, we are increasingly surrounded by complex systems like Pickering-Ramsden emulsions, which are present in a wide array of products from food and cosmetics to pharmaceuticals and cutting-edge nanotechnology. Unlike traditional emulsions, which rely on conventional emulsifiers, Pickering emulsions are stabilized by solid particles, offering a novel and more stable approach to emulsion formation. This particle-based stabilization provides significant advantages, including enhanced stability and the potential to tailor functional properties like mechanical strength. Pickering emulsions exhibit complex rheological behaviors, making the prediction of their flow, deformation, and stability a significant challenge. Therefore, the precise role of interfacial particles in influencing the overall behavior of these emulsions remains inadequately understood.

In this study, the underlying complexities of the interfaces were investigated to address key gaps in understanding how particle-loaded droplet properties, and flow conditions are affected by interfacial rheology. Our approach focused primarily on experimental methods, with computational models used later to predict the behavior of particle-coated droplets. Interfacial (2D) and bulk (3D) rheology were used to characterize the mechanical response of the particle-laden fluid-fluid interfaces and particle-coated droplets under deformation and flow. High-resolution microscopy revealed that the particle distribution at the interface is highly sensitive to several factors, including surface coverage, particle size, and wettability. While the distribution appeared more homogeneous under certain conditions, it became heterogeneous when these factors were manipulated.

Langmuir trough experiments showed that surface pressure increased nonlinearly with compression, suggesting interactions already at moderate surface coverages. State-of-the-art 2D rheometry revealed that higher surface coverage led to enhanced interfacial viscosity and modulus, in addition to introducing a yield stress, indicating the formation of a more elastic, jammed interfacial network. This behavior at the interface leads to enhanced stability, confirming the mechanical coupling between interfacial and bulk phases.

**Keywords:** Pickering-Ramsden emulsion, interfacial and bulk rheology



**Figure 1.** Schematic representation of a Pickering-Ramsden emulsion from macro to micro scale perspective.



## Interface stabilization mechanisms: Insights from the Dynamic Thin Film Balance (DTFB) technique

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Thin liquid films (TLFs) formed between bubbles/droplets in proximity are ubiquitous and govern the macroscopic stability & lifetime of emulsions/foams, critical to designing products for diverse applications. The dynamic thin film balance (DTFB) is a versatile technique that can be used to study the drainage & rupture of emulsion/foam films, with the advantage of monitoring film behaviour at length (microscopic) scales observed in real systems. This technique with precise pressure control can effectively bring out structural forces arising under confinement of molecules in real time. This method offers the advantages of uniform radial drainage, high operating pressures and reusability but poses some challenges as well. Its functional design can be used for Pickering foams/emulsions but is limited by the size of the particle, owing to the diameter of the bike-wheel and the channels. Since this technique uses interferometry for thickness determination, the resolution depends on the difference in refractive indices across the interface. While it provides high precision measurement at air-water interface, measurements at liquid-liquid interface remain a challenge, stemming from small differences in refractive index. The future scope lies in modifying the bike-wheel design to make it suitable for larger particles ( $\mu\text{m}$ ). Fluorescence-based methods can enable the study of liquid-liquid interfaces and help visualize interfacial stresses. We aim to highlight the significantly different mechanisms by which foam films drain and rupture based on the type of stabilizing molecule (surfactant, polymers/proteins, colloidal particle) ranging from DLVO forces to non-DLVO forces for films with macromolecules showing time dependent adsorption. The differences in thinning mechanism, drainage and rupture of TLFs are thus an interplay between the type of stabilizing molecule, charge, polydispersity, flexibility of molecules & nature of the adsorbed species.

**Keywords:** Dynamic thin film balance, thin liquid films, macroscopic stability

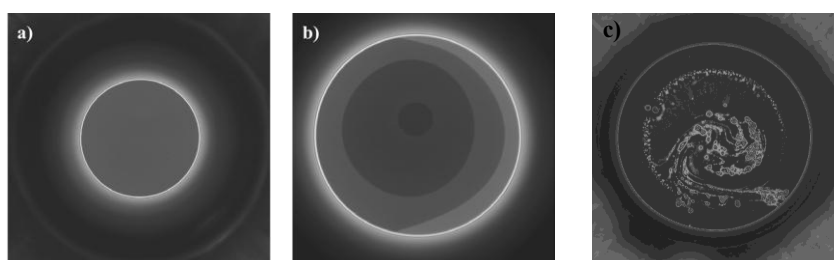


Fig 1. Thinning of a) SDS stabilized TLFs below CMC and b) above CMC (stepwise thinning called Stratification) c)  $\beta$ -lactoglobulin stabilized film

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## Binding Affinity Controls Ion Transfer in Tribocharging

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The driving force for charge transfer during contact electrification has been debated as a product of either electron transfer, ion transfer, or material transfer. While it has been demonstrated that electron transfer occurs between conducting metals through differences in work functions, the driving force for similar charge transfer in polymeric materials remains uncertain.[1] In order to elucidate the roles each type of transfer may play in contact electrification, this work specifically evaluates the role of ion transfer through ionomer surface modified materials. Immobile charged groups with a mobile counter ion species were introduced to the surface of polydimethylsiloxane samples (PDMS), which then transfer charge during contact with counter PDMS samples. It's been shown that bound charged groups with mobile counter ions transfer charge to a counter sample which corresponds to the sign of charge of the mobile species.

With one fixed charge group, a series of mobile ions were introduced to evaluate the impact on charge transfer. Initial work has focused on the introduced a sulfonic acid moiety that is associated with mobile ions of Na<sup>+</sup>, K<sup>+</sup>, and Li<sup>+</sup>. We have demonstrated that the charge transfer is higher for Li<sup>+</sup> compared to K<sup>+</sup>. This matches the proposed Hofmeister series trends which suggests that sulfonic acid groups have a stronger affinity towards K<sup>+</sup> and a weaker affinity towards Li<sup>+</sup>. [2] Na<sup>+</sup> is the middle point of the Hofmeister series, and our experimental data confirmed this as well.

A second ionomer moiety was studied to further quantify the effect of binding affinity on charge transfer. A carboxylic acid moiety was chosen as this sits on the opposite side of the Hofmeister series, which predicts that stronger affinity occurs towards Li<sup>+</sup> and weaker affinity to K<sup>+</sup>. Our experimental results conclusively demonstrate. This work helps elucidate the role that ions play during contact electrification.

**Keywords:** Contact Electrification, Ionomers, Hofmeister Series

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## **Electrokinetic Transport at Microfluidic Interfaces: From Electrowetting to SAW-Driven Double Layer Dynamics**

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Electrokinetic transport near microscale interfaces plays a central role in a wide range of applications, from droplet actuation and wetting control to charge manipulation in confined geometries. In this study, we present two complementary modeling strategies, both rooted in the Poisson–Nernst–Planck–Stokes (PNPS) framework, to investigate field-driven electrohydrodynamics in distinct but physically related settings. The first part focuses on a diffuse-interface formulation for immiscible electrolytic systems, where interfacial dynamics are resolved using a phase-field approach coupled to ionic transport and fluid flow [1]. This model captures key nonlinear effects such as contact angle saturation and electrowetting hysteresis, and is particularly suited for describing microscale two-phase systems subjected to electric forcing. In contrast, the second part addresses the dynamic response of a single-phase electrolyte solution under high-frequency surface acoustic wave (SAW) excitation [2,3]. Here, we analyze the electrohydrodynamic resonance of electrical double layers (EDLs) by combining boundary-layer theory with linear perturbation analysis. The model reveals how acoustic streaming drives charge redistribution near solid surfaces and leads to enhanced electrokinetic flows. Although the two systems differ in geometry and dominant physical mechanisms, both share a consistent thermodynamic basis and highlight the versatility of the PNPS framework in capturing electrokinetic coupling across fluid – fluid and fluid–solid interfaces. Numerical results from each model illustrate characteristic behaviors—such as fieldmodulated wetting, ion accumulation, and resonance amplification—that have direct relevance for microfluidic control, interfacial design, and energy conversion technologies.

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## Study of Giant Unilamellar Vesicles' Fluidity

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In this study, we examine the effect of microgravity on the membrane fluidity of giant unilamellar vesicles (GUVs) made of DOPC and Cholesterol. GUVs are prepared using electroformation technique, during which a thin film of lipids is deposited on a conductive glass substrate while the application of AC electric field accelerates the swelling of the lipid film. We first study the fluidity of the vesicles over a range of DOPC/Cholesterol ratios using Fluorescence Recovery After Photobleaching (FRAP): a disk shaped area of the vesicle is bleached using a laser for a short amount of time and the fluidity is computed from the time of fluorescence-recovery time. The same fluidity also is investigated by means of fluorescence polarization anisotropy (FPA) technique, where the intensity of the sample's fluorescence emission is measured along two orthogonal polarization axes. The latter method can be implemented under microgravity conditions. We report a significant fluidity changes in microgravity conditions, where the vesicles display approximately 20% higher membrane fluidity compared to those measured on the ground. Our findings provide valuable insights on the cells' behavior in zero-gravity conditions and more specifically about the absorption of pharmaceuticals in the human body.

**Keywords:** vesicles, lipids, membrane, fluidity





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## **Role of cholesterol on structural and mechanical properties of lipid monolayer at the water-air interface**

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In modern society, due to industrialization and increasing climate change, the amount of micro- and nano-pollutants in the air and water is dangerously rising. Those pollutants easily affect the human organisms especially where directly expose to outer environment.

In this project, we investigate the structural and mechanical properties of model lung surfactants in the presence of active and passive microparticles. As experimental model, Dipalmitoylphosphatidylcholine (DPPC) and Cholesterol (Chol) are used. Langmuir-Blodgett trough monitors lipid monolayers during compression, while fluorescence microscopy visualizes the domains. Rheology is measured at various frequencies using an interfacial shear rheometer coupled with trough.

The presence of cholesterol in DPPC monolayers results in monolayers with higher elasticity, an effect that can be explained by cholesterol's steroid groups being situated between the hydrophobic tails of DPPC lipids. During compression, pure DPPC monolayers transition from LE to LC, with a plateau at surface pressure  $\Pi = 5\text{--}6$  mN/m and collapse at  $\Pi = 60\text{--}65$  mN/m. The domain shape changes from round to fractal. Adding Chol lowers the collapse pressure ( $\Pi = 45\text{--}50$  mN/m) and eliminates the plateau when Chol exceeds 8.6 mol %. Rheology shows that Chol decreases surface viscosity and makes the monolayers more elastic at higher frequencies. This result was confirmed by fluorescence imaging of a structure of lipid domains. The average size was decreased by Chol concentration while connectivity was increased.

The presence of SiO<sub>2</sub>-NH<sub>2</sub> fluorescence particles in DPPC monolayer also showed the similar results.

**Keywords:** Lipid monolayer, isotherm compression, Lipid domain



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## Enhancing porosity in supraparticles: A simulation study using spherical filler particles and rod-shape particles

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Supraparticles (SPs) are large assemblies of smaller colloidal particles, whose properties can be tuned by modifying, e.g., the chemistry, shape, and size of the individual constituent particles and their arrangement within the SP. SPs can be formed through droplet drying, a process commonly observed in both everyday life and industrial applications, such as aerosol droplets, spray drying, and printing. Porous SPs are of particular interest, since their high surface area and tunable pore size distribution makes them ideal materials for catalysis, photonics, and adsorption applications. In this computational study, we explored the drying-induced formation of SPs made from spherical filler particles and rod-shaped particles. After drying, we remove the filler particles to reveal a highly porous structure. The volume fraction between spherical and rod-shaped particles plays a key role in shaping the porosity within the SP, while increasing the aspect ratio of the rods further amplifies the porosity of SP. Additionally, we observed that slower drying rates lead to a distinct increase in average pore size. These insights into increasing the porosity through particle size, shape, and drying conditions provide a valuable framework for designing highly porous SPs.

**Keywords:** Supraparticles, Drying induced assembly, Rod-shape particles



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## i-Combisomes: a versatile platform for synthetic cell membranes

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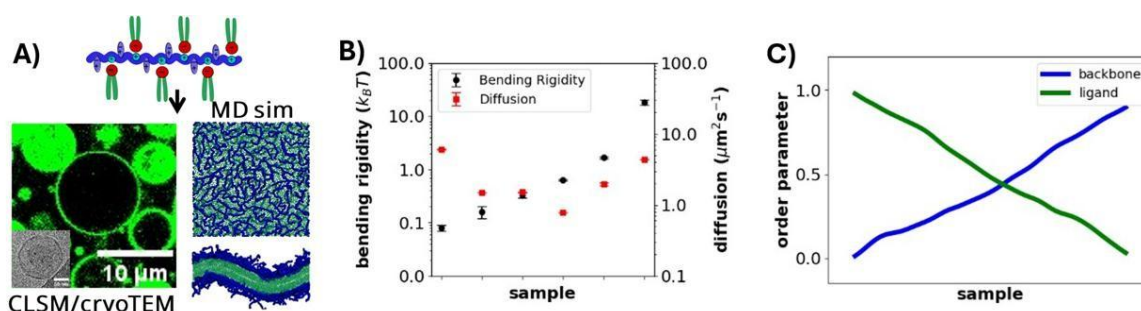
We recently introduced ionically linked comb polymers (iCPs) [1–2] which are supramolecular macromolecules consisting of a hydrophilic backbone with cationic groups to which anionic surfactants are appended. In water they self-assemble into giant vesicles called i-combisomes. These vesicles have membrane that mimics some of the key properties of the cell membrane. The membrane comprises an inner surfactant bilayer, flanked on both sides by 2D cationic backbones. These backbones can exhibit nematic-like ordering (Figure 1A), positioning i-combisomes between polymersomes and polyelectrolyte–surfactant complexes in terms of structural classification.

Due to their unique topology, i-CPs allow for a wide range of modifications, resulting in high diversity in both dynamic and static membrane properties of the i-combisomes that they form. Using molecular dynamics simulations, we show that by varying the backbone (e.g., the ratio of cationic monomers and degree of polymerization) and surfactant structure (e.g., number and length of tails), the bending rigidity can be tuned across nearly two orders of magnitude, from highly flexible ( $\sim k_B T$ ) membranes to stiff ones ( $\sim 100 k_B T$ ), comparable to polymersomes. In contrast, the lateral diffusion coefficient remains within a narrow range, similar to that of liposomes (Figure 1B).

These properties are tightly coupled to the balance between backbone and surfactant ordering (Figure 1C). This balance is defined by the charge distribution of the cationic monomers in the polymer layer and the spatial arrangement of the surfactant head groups, which is in turn mediated by tail organization.

Our findings highlight i-combisomes as a highly promising platform for artificial cells, fundamental biophysical studies, and technological applications.

**Keywords:** synthetic biomembranes, polyelectrolyte-surfactant complexes, molecular dynamics



**Figure 1.** A) Self-assembly of iCPs, B) mobility-dependent parameters of vesicles, C) schematic representation of backbone and ligand ordering.

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## Mechanical Durability of Fluorinated and Non-Fluorinated Silicone-Based Polymer coatings

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Mechanical stability of polymeric coatings is a necessary property for the utilization of these materials in certain applications. In this work, the mechanical durability and surface characteristics of fluorinated and non-fluorinated silicone-based polymer coatings are investigated. The coatings are applied to both stainless steel and polypropylene substrates. The effect of the development of nanocomposite coatings by incorporating various additives like Al<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> nanoparticles, as well as layered materials like MXene on the mechanical performance of the coatings was systematically studied, as well. Abrasion resistance was evaluated through standardized tests, with the coatings subjected to up to 2500 abrasion cycles.

The result of abrasion on the various coated surfaces was evaluated using Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), contact angle measurements, and Atomic Force Microscopy (AFM). In most cases, the polymer coatings exhibited resistance to surface wear and maintained their hydrophobic properties after the abrasion test. To enhance abrasion resistance, the addition of an appropriate binder between the substrates and the polymer and/or the inorganic nanoadditives is investigated.

**Keywords:** Abrasion, Mechanical durability, Polymer coatings, Nanocomposites

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## Development of Non-Fluorinated Superhydrophobic Polymer Coatings

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Superhydrophobic and water-repellent surfaces that exhibit high water contact angles and low contact angle hysteresis are defined by their chemistry and an appropriate hierarchical roughness. These surfaces have gained a lot of attention due to their self-cleaning properties that make them candidates for a plethora of applications. In the majority of the cases, these surfaces depend on fluorinated polymer coatings, the use of which is increasingly prohibited due to their harmful effects on health and the environment.

This work investigates the development of a sustainable alternative to fluorinated coatings that are based on Protectosil WS 610 which is a siloxane polymer emulsion. The coatings were deposited through dip-coating on various substrates, including glass, stainless steel and polypropylene. Moreover, spraying the coated surface with alkaline aqueous solution was necessary for the formation of a homogenous film. To attain the appropriate hierarchical roughness, nanoadditives like SiO<sub>2</sub> and TiO<sub>2</sub> nanoparticles, along with 2D Mxene nanosheets, were added to the polymer matrix. Surface properties were assessed via contact angle and contact angle hysteresis measurements, along with scanning electron microscopy (SEM). Moreover, abrasion resistance and thermal stability tests were performed to assure the durability of the coatings, whereas cytotoxicity measurements certified their safe use in applications involving human interaction. Optimal coatings had contact angles exceeding 150° and low roll off angles. The coatings exhibited uniform performance on all examined substrates, indicating their suitability for various applications. These findings indicate that these siloxane-based systems present a practical, eco-friendly substitute for fluorinated coatings, with possible applications in self-cleaning surfaces, pollution-resistant materials, and sustainable coatings.

**Keywords:** Superhydrophobic coatings, Fluorine-free surfaces, Water repellency, Siloxane polymers



**Figure 1.** Water repellence of a stainless steel substrate coated with a nanohybrid film consisted of Protectosil WS 610 and SiO<sub>2</sub> nanoparticles following thermal annealing.

**Acknowledgements:** This research has been partially financed by the EU Horizon Europe Programme (project STOP, Grant Agreement 101057961).

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## Molecular Understanding of Soil-Fabric Interactions for Sustainable Textile Care

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This research explores the significant implications of climate change, with a focus on the 2050 Net Zero goal, specifically within the domain of textile care. A key strategy in achieving this goal involves minimizing water consumption, reducing wash cycle temperatures, whilst maintaining the lifespan of the garment. Complex organic soils (COS), composed of lipids, proteins, sugars, and metal ions, present a significant challenge in cleaning. Their residues require repeated washing, leading to increased water and energy consumption, contributing to textile waste in landfills. The interactions of COS components, with fabric surfaces is relatively unknown and presents a considerable hurdle in understanding effective soil removal. To understand their interactions on a molecular level, a library, of key lipid constituents of sebum, a major component of COS has been deuterated.[1] These targeted lipids include fatty acids, triglycerides, wax esters, and cholesterol, which are known to play a crucial role in soil adhesion and persistence.

Furthermore, a novel flow FTIR-ATR system has been developed in conjunction with the synthesised molecular probes. This deuteration process ensures minimal alteration to the physical properties, while enabling the C-D stretches of the molecular probes to be monitored and tracked throughout a wash cycle. This allows for a better understanding of the mechanisms governing soil removal, the interactions between different soil components, and provides an in-situ analytical tool for monitoring soil removal and evaluating various formulation conditions.[2]

A detailed understanding of the residues responsible for fabric staining, and soil accumulation is crucial for the design of formulation components enabling efficient soil removal, reducing textile waste that contributes to landfill challenges. This study enhances fundamental understanding of the interactions between soil components, fabric surfaces, and cleaning solutions, ultimately working towards a Net Zero future.

**Keywords:** Flow FTIR-ATR, deuteration, soil-textile interactions

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## Unveiling the Structural Evolution of Lipid Liquid Crystalline Nanoparticles: The Role of Functionalization

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Lipid-based liquid crystalline nanoparticles (LLCNPs) are versatile platforms for drug delivery and bioimaging, and their structural organization directly governs loading capacity, release kinetics, and biological interactions. Using complementary characterization techniques—small-angle X-ray scattering (SAXS), cryogenic transmission electron microscopy (cryo-TEM), and dynamic light scattering (DLS)—we demonstrate how functional groups, modification with nanoparticles of various characteristics, and mixing different lipids influence phase behavior, lattice parameters, and interfacial curvature.

LLCNP colloids can be prepared using different structure-forming lipids, for instance, glyceryl monooleate (GMO) and phytantriol (PHT), either separately or by mixing them with other bioactive compounds exhibiting specific functionalities, such as glyceryl monolaurate (GML) [1, 2]. In this way, it is possible to produce a wide range of structures with varying arrangements.

The complex structure of LLCNPs is also significantly disrupted when inorganic nanoparticles, such as MnO, are introduced as MRI contrast agents [3]. Modifying Gd-chelating lipids appears to be a safer approach for obtaining low-toxicity materials; however, their distinct structure causes rearrangement of LLCNPs, potentially leading to less ordered or different molecular arrangements compared to the commonly observed cubic phase [4]

**Keywords:** lipid nanoparticles, biomedical applications

**Acknowledgements:** IDUB International Research Team project, BioSoft – Soft Matter for Bioimaging and Regenerative Medicine, 173/02/UAM/0036

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# M. Experimental & Computational Methods (including AI)



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## Reverse mapping from DPD model to all-atom MD model of star polymer self-assembled structure

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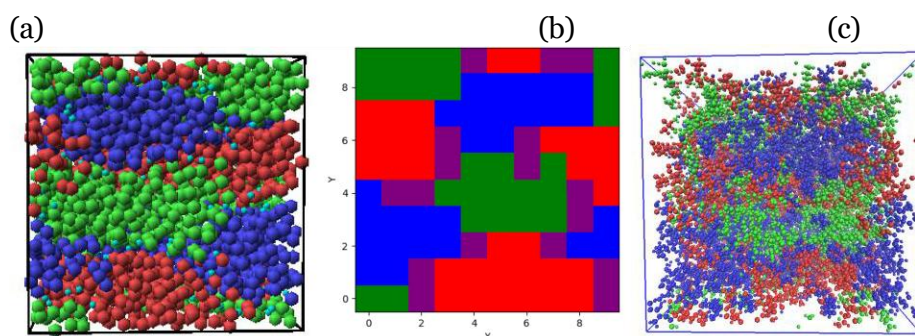
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Molecular simulation is a method for calculating the molecular motion and analyzing structure and physical properties, and a typical example is molecular dynamics(MD). MD is a method that calculates the motion of all atoms and is used for detailed materials analysis at the microscopic scale. Although MD is widely used in materials research due to its high analytical accuracy, it is computationally expensive and difficult to analyze on a large scale and over a long period of time. Therefore, coarse-grained (CG) simulations of mesoscale structures are expected to evaluate large scales such as polymers or phase separation behavior. Several models and methods have been proposed for CG methods, such as dissipative particle dynamics(DPD), but they cannot directly calculate atomic interactions at the microscale. Accordingly, reverse mapping has been developed to recover microscale structures from CG models.

Reverse mapping enables MD calculations at larger scales, such as phase separation and polymers, by reconstructing atomic configurations from CG models. Although reverse mapping methods have been developed to suit specific models [1], multiple issues must be considered, such as atomic interactions and polymer entanglement. Therefore, current applications are often limited to relatively small or constrained systems, such as a single water molecule or rigid polymers. There is a need for a general-purpose reverse mapping method that can be applied to a variety of molecules and complex structures.

In this study, we developed a reverse mapping method that can reproduce phase-separated structures formed by star polymers with complex structures such as multiple branches. First, we evaluated the self-assembled CG structure of star polymers using DPD simulations. Next, we divided the simulation space based on the local concentration of model types to define the reverse mapping region. Finally, we placed an all-atom model of the star polymer within this region to reconstruct the MD model.

**Keywords:** Reverse mapping, DPD, MD, Self-assembly, phase separation



**Figure 1.** (a) Screenshot of star polymer DPD structure. (b) reverse mapping region. (c) reconstructed MD structure

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## Recognizing and generating knotted molecular structures by machine learning

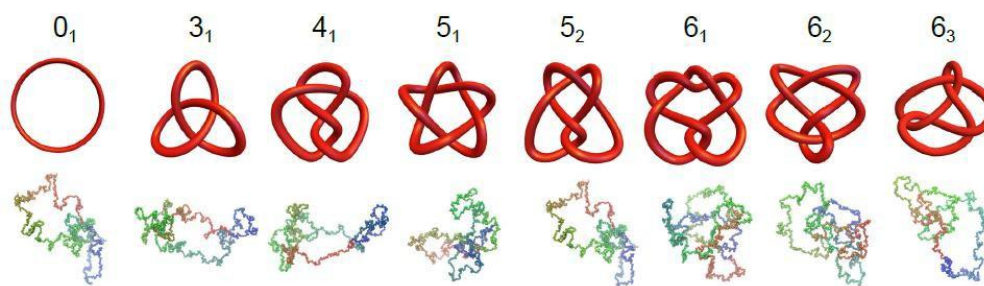
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Knotted molecules occur naturally and are designed by scientists to gain special biological and material properties. Understanding and utilizing knotting require efficient methods to recognize and generate knotted structures, which are unsolved problems in mathematics and physics. Here, we solve these two problems using machine learning. First, our Transformer-based neural network (NN) can recognize the knot types of given chain conformations with an accuracy of >99%. We can use a single NN model to recognize knots with different chain lengths, and our computational speed is about 4500 times faster than the most popular mathematical method for knot recognition: the Alexander polynomials. Second, we for the first time design a diffusion-based NN model to generate conformations for given knot types. The generated conformations satisfy not only the desired knot types, but also the correct physical distributions of the radii of gyration and knot sizes. The results have several implications. First, the Transformer is suitable for handling knotting tasks, probably because of its strength in processing sequence information, a key component in knotting. Second, our NN can replace mathematical methods of knot recognition for faster speed on many occasions. Third, our models can facilitate the design of knotted protein structures. Lastly, analyzing how NN recognizes knot types can provide insight into the principle behind knots, an unsolved problem in mathematics. We provide an online website (<http://144.214.24.236>) for using our models.

**Keywords:** Artificial Intelligence, Knot, Topology, Polymer







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## Unveiling force relaxation mechanisms in a protein-based hydrogel

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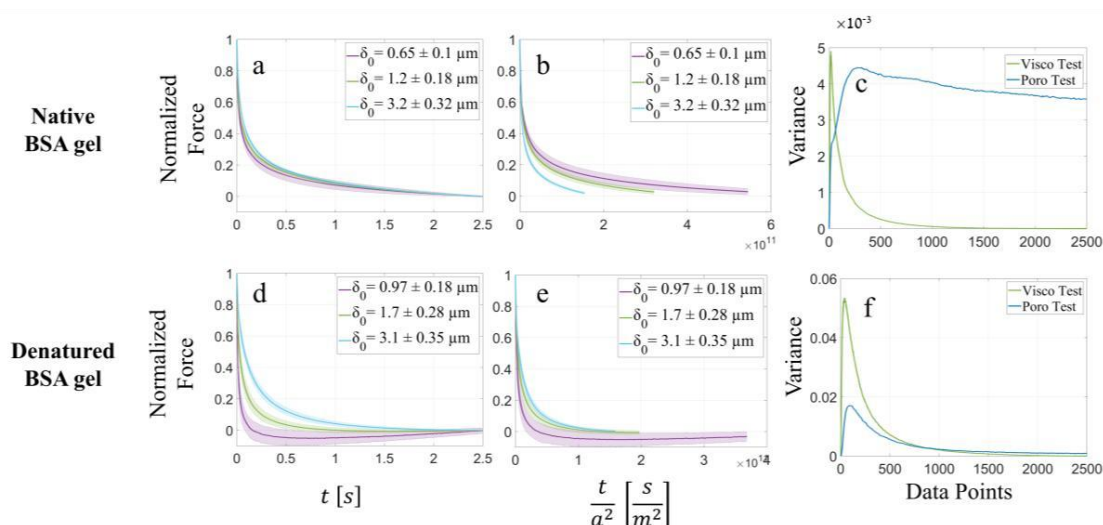
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Protein-based hydrogels (PBHs) have attracted significant attention as materials capable of exhibiting enhanced mechanical properties. The appeal of these materials lies in the ability of their constituting proteins, that have a well-defined 3D native structure, to unfold under force application and refold when the force is removed. Consequently, PBHs display distinct mechanical response to load that reflect the inherent properties of their protein building-blocks, including stiffness, stretchability, and stress relaxation behavior. Nevertheless, the underlying mechanisms that govern the mechanical behavior of PBHs are still not fully characterized. Here, we study the nature of the time-dependent mechanical force response of bovine-serum albumin (BSA)-based hydrogels. Using Atomic Force Microscopy (AFM) indentation and force-relaxation measurements, we distinguish between two mechanisms – viscoelasticity, where the material's relaxation time is independent of the strain length-scale, and poroelasticity, which demonstrates a clear dependency on this parameter. Our analysis of stress relaxation force traces reveals that the BSA-PBH's dissipative mechanism is predominantly viscoelastic, resulting from slow dissipation processes within the hydrogel associated with protein conformational changes and internal friction between side chains. In contrast, when placed in a denaturing environment where proteins are completely unfolded, the same BSA-PBH exhibits poroelastic dissipation, indicating that energy dissipation is controlled by the interaction between fluid movement and matrix displacement within the hydrogel. These findings highlight the role of protein structure in defining PBH mechanical behavior and scalability.

**Keywords:** hydrogel, protein-based hydrogels, viscoelasticity, poroelasticity.



**Figure 1.** Normalized force vs. time of BSA hydrogel in native (a) and denatured (d) states. Normalized force vs. lengthscaled time of BSA hydrogel in native (b) and denatured (e) states. Comparison of the variance in both the graphs of the viscoelasticity check and the poroelasticity check for BSA hydrogel in native (c) and denatured (f) states. Convergence in plots (a) and (e), evident also by lower values of variance in (c) and (f), indicate viscoelastic and poroelastic behaviors, respectively.



# P. Polymers and Networks (including Sustainable Soft Matter)

## Thermal elasticity of disordered underconstrained systems

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Underconstrained systems possess more degrees of freedom than constraints and are widely used to model the rigidity of disordered biological materials, such as spring networks for biofiber gels and vertex models for biological tissues. At zero temperature, Maxwell counting predicts that these systems are typically floppy. However, they can be stiffened either by applying external strain or by introducing finite temperature. In the athermal case, strain-induced stiffening has been attributed to the emergence of a state of self-stress (SSS) — a force-bearing structure in which non-zero tensions from constraints (e.g., springs) balance to produce zero net force at local connecting nodes. While the role of SSS in athermal stiffening is well studied, its influence in the thermal regime remains less understood. Here, we extend our previous SSS theory for athermal systems [1,2] to incorporate finite-temperature effects [3,4]. Near the stiffening transition, we derive from first principles analytic expressions for elastic properties, such as isotropic tension  $t$  and shear modulus  $G$ , and clarify their dependence on temperature  $T$ , isotropic strain  $\varepsilon$ , and shear strain  $\gamma$ . These expressions involve only three parameters that are extractable from the SSS: the entropic rigidity  $\kappa_s$ , the energetic rigidity  $\kappa_E$ , and a coupling parameter  $b_e$  describing the interaction between isotropic and shear strains. Our results reveal that underconstrained systems behave like two springs in series (with one entropic spring and the other energetic), providing a simple explanation for the previously observed numerical scaling  $t \sim G \sim T^{0.5}$ . Given its generality, our theoretical results should be applicable to a broad class of underconstrained materials.

**Keywords:** thermal elasticity, amorphous, state of self-stress

**Acknowledgements:** The project leading to these publications [2-4] has received funding from France 2030, the French Government program managed by the French National Research Agency (ANR-16-CONV-0001), and from the Excellence Initiative of Aix-Marseille University - A\*MIDEX.

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## Tuning the Rheology of PDMS Inks with Gelatin Hydrogels for Advanced 3D Printing

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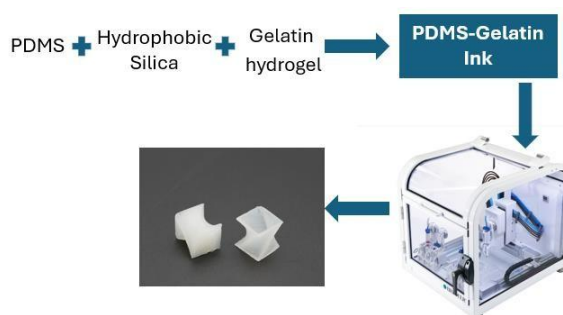
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Polydimethylsiloxane (PDMS) is a widely used elastomer in soft robotics, biomedical devices, and microfluidics due to its flexibility, biocompatibility, and chemical stability. However, its low viscosity and poor printability pose significant challenges for direct ink writing (DIW) in 3D printing.

Traditional approaches to improve the rheological properties of PDMS inks involve the addition of fillers, such as silica particles, which increase yield stress but often result in rigid final structures [1]. Other approaches used to change the rheological properties of PMDS include the addition of liquid fillers or a combination of liquid and solid fillers, resulting in emulsions or capillary suspensions, respectively [2], [3]. In this study, we investigate the effect of gelatin hydrogel on the rheological properties and 3D printing ability of the PDMS inks.

Gelatin, a biopolymer derived from collagen, offers tunable viscoelastic properties and thermal responsiveness, making it a promising additive for ink formulation. By combining the gelatin hydrogel with a reduced amount of silica particles, a 2-fold increase in viscosity is observed. Furthermore, we demonstrate the ability of the materials to be extruded into complex shapes.

**Keywords:** Gelatin, PDMS, 3D printing,



**Figure 1.** Schematic figure showing the printing process of the PDMS-gelatin hydrogel inks.

**Acknowledgements:** The authors express their sincere gratitude for the funding provided by the Novo Nordisk Foundation through the Challenge Program, grant number NNF22OC0071130.

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## Understanding Freeze-Fracture in Soft Model Hydrogels

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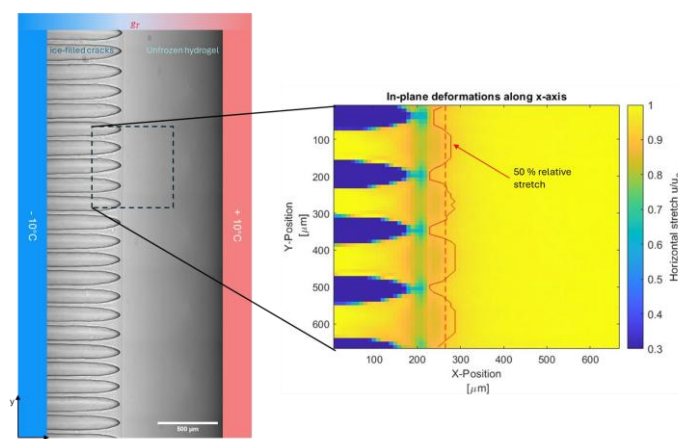
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Freezing-induced damage in soft, porous materials is a widespread problem that is still poorly understood, but which impacts many disciplines such as geology, and material and food sciences [1]. There are two key problems that have made it hard to make progress on this problem. Firstly, most samples of interest are not transparent, so it is hard to directly visualize freezing damage processes. Secondly, materials like food, tissue and clay have complex fracture properties, and so they break in complex ways. Here, we develop a model freezing system, using transparent hydrogels. When we freeze these gels at a constant rate, we observe the formation of beautifully periodic, ice-filled cracks (Fig. 1 (left)). These provide an excellent testbed to understand the freeze-fracture process.

Our experimental setup allows us to systematically vary experimental conditions and identify underlying physical parameters driving freeze damage. In particular, we observe that changing the freezing speed, the sample thickness and the temperature gradient lead to different freezing crack shapes and spacing between the cracks. We explain why these parameters control the freezing damage, and show how freezing damage is caused by the shrinking of the gel due to desiccation: a consequence of 'cryosuction' that pulls water out of the gel towards the growing ice cracks.

**Keywords:** Soft Hydrogels, Fracture, Freezing, Dehydration



**Figure 1.** (left) Microscope image of ice-filled cracks in a PEGDA hydrogel growing inside a temperature gradient, while the sample moves at a constant speed. (right) Stretch map of the horizontal in-plane stretch along the x-axis from PIV Data.

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## Viscoelasticity of Vitrimer Melts and Solutions

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Vitrimers uniquely combine the advantageous properties of both thermoset and thermoplastic materials. Their defining characteristic is the presence of dynamic covalent bonds, which exhibit an Arrhenius temperature dependence.

This study investigates the linear viscoelastic (LVE) behavior of well-characterized model polyisoprene vitrimers and their solutions, providing insights into the complex interplay between chemical dynamics and mechanical responses. We explore the evolution of storage and loss moduli across various frequencies and temperatures, focusing on the strong time dependence and the role of cluster formation of the bonding motifs. LVE master curves are formed and compared against the respective precursors, revealing the dramatic extent of the plateau region and the distinct signature features of these materials. These features are shown to be tailored by systematically changing the molecular weight of the precursor. The vitrimer networks exhibit a gradual transition from elastic behavior to viscoelastic flow, driven by the activation of bond exchange reactions.

These findings open avenues for the design of next-generation vitrimers and their application as compatibilizers for innovative blends with adjustable mechanical properties, facilitating transformative possibilities in self-healing materials, sustainable manufacturing, and more.



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## Shear Induced Tuning of Mechanical Properties and Ionic Conductivity of Composite Polymer Electrolytes

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Composite polymer electrolytes have been shown to be promising candidates to enhance the poor mechanical properties of conventional polymer electrolytes. Many inorganic particles have been tested in order to induce percolation inside the composite electrolyte and provide mechanical stability. Even though the effect of the addition of inorganic particles on the ionic conductivity has been previously studied, little attention has been given to the effect of the morphology of the network itself. In this work, composites are synthesized using low molecular weight poly(ethylene) glycol ( $M_r=500$  g/mol), hydrophobic fumed silica and Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), a system known to have shear history effects. Rheology is used to induce structural changes to the network formed by the fumed silica, through steady preshear. We combine this with a custom-made Rheo-Electrochemical Impedance Spectroscopy setup to measure the conductivity of the composite electrolyte in-situ, and thus, correlate the conductive pathways of the ions with the microstructure. We find that the addition of the inorganic particles has negligible effects on the ionic conductivity due to the open, fractal structure formed by the fumed silica and that conductivity is independent of the applied preshear, even though the storage modulus of the gel created varies almost an order of magnitude.

**Keywords:** battery, composite polymer electrolytes, preshear



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## Synthesis and Characterization of Novel Polymeric Photoresists for Green Lithographic Processing

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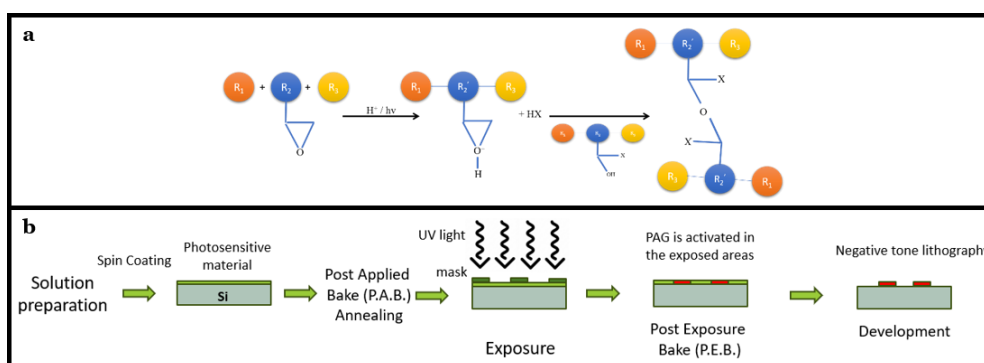
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Semiconductor lithographic technology has received growing attention due to its interesting and wide range of industrial applications. The massive need to reduce the integrated circuits dimensions has created the need to discover new lithographic techniques for high volume manufacturing. However, the environmental challenges, related to semiconductor manufacturing and more specifically to the reduction of their environmental footprint, are significant. The use of highly toxic and environmentally harmful solvents, especially during the resist coating and development process steps constitutes a major drawback in the lithographic technology.

Herein, we present the development of new polymeric photoresists which allow the elimination of the use of organic solvents and aqueous alkaline solutions that are currently being used in the lithographic process. Our aim is to replace the organic solvents and highly alkaline TMAH solutions used in spin coating and in the material development, respectively, with water. A variety of organic/hybrid polymeric materials were synthesized and evaluated chemically amplified photoresists. The polymers comprised two, three or four comonomers in various combinations and compositions, in order to meet the required material properties such as solubility in water, stiffness, absorptivity and high glass transition temperature. Simultaneously, the use of photoacid generators (PAGs) was necessary to cross-link the materials during UV ( $\lambda = 254\text{nm}$ ) exposure (Figure 1.a) and tune the solubility in the exposed areas forming the final photoresist pattern (Figure 1.b).

**Keywords:** green photoresists, lithography, water-soluble polymeric materials



**Figure 1.** Schematic illustration a) of the cross-linking mechanism and b) the spin coating and negative lithographic processing.

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## Dual pH- and Thermo- Responsive Poly(amido amine)s with a Critical Temperature in Aqueous Media

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The “smart” behavior of stimuli-responsive polymers has led to remarkable success over the past few decades, driven by their promising applications ranging from drug and gene delivery and tissue engineering, to environmental sensing and others. Among the various stimuli employed, temperature has gained significant attention and has been often coupled with additional stimuli, such as pH and light, to enable an enhanced control over the physicochemical properties of the polymers [1]. However, to impart degradability, a valuable characteristic for biomedical and environmental applications, on stimuli-responsive polymers, post-polymerization reactions of degradable polymers are often required, which render the process demanding and challenging [2].

Herein, we describe the temperature-responsive behavior of poly(amido amine)s, a well-established class of biocompatible, pH-responsive, and degradable polymers, which were synthesized via a facile one-step aza-Michael polyaddition of amines to bisacrylamides [3]. The polymers were characterized by size exclusion chromatography and <sup>1</sup>H NMR spectroscopy, while their cloud points were determined by turbidimetry in aqueous media. By modulating the hydrophilic to hydrophobic balance within the poly(amido amine)s backbone, via the incorporation of hydrophilic or hydrophobic primary amine comonomers, we uncovered a tunable lower critical solution temperature-type thermo-responsive behavior with sharp phase transitions. The critical solution temperature of the polymers was found to depend on the polymer molecular weight and its concentration in solution as well as the solution pH. Finally, end-functionalized poly(amido amine)s that bear either amine or activated double bonds were accessed, which can be further employed to develop complex degradable, thermo-responsive polymer architectures. The present work paves the way towards the synthesis of novel degradable, dual pH- and thermo-responsive polymers via a facile approach, which employs commercially available comonomers.

**Keywords:** pH-responsive, thermo-responsive, degradable polymers

**Acknowledgements:** This research was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the “2nd Call for H.F.R.I. Research Projects to support Faculty Members & Researchers” (Project Number: HFRI-FM17-3346).

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## Recyclable organogels from thermosetting polydimethylsiloxane with light-triggerable bonds

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Organogels are a class of materials comprising cross-linked polymers or supramolecular networks swollen in organic solvents. Their functional diversity and unique characteristics—such as thermal and mechanical stability, surface wettability, and stimuli-responsive behavior—render them ideal candidates for a wide range of applications, including drug delivery systems, actuators, oil–water separation membranes in food processing, wearable electronics, and recyclable materials [1,2]. Light-induced organogel degradation relies on photo-labile bonds located either on the main chain of the polymer or at the cross-link points of the network [3-5]. Despite the abundance of labile bonds, organic solvents, and compatible networks that offer a wide range of properties, relatively few studies have been conducted in this area.

Herein, we present a new class of light-degradable networks bearing thioacetal cross-link junctions, which undergo photocleavage upon UV light irradiation in both the swollen and dry state. The organogels were synthesized via an acid-catalyzed cross-linking reaction of a difunctional polydimethylsiloxane (PDMS)-dithiol or PDMS-dialdehyde precursor polymer with terephthalaldehyde or 1,4-benzenedimethanethiol, respectively. The chemical structure of the synthesized gels was confirmed by solid-state  $^1\text{H}$  and  $^1\text{H}-^{13}\text{C}$  HSQC NMR and FTIR spectroscopies, while their viscoelastic behavior was investigated using dynamic shear rheology.

The photo-induced cleavage of the labile bonds was studied under UV light irradiation ( $\lambda = 254$  nm, intensity =  $0.063 \text{ mW cm}^{-2}$ ), which showed a complete degradation of the swollen gels within 2 hours, whereas the dry network exhibited ~30% mass loss for the same irradiation time (Figure 1). As a new addition to the library of photodegradable organogels, the proposed system is expected to open up further opportunities for the development of novel functional recyclable materials across a wide range of applications.

**Keywords:** UV-irradiation, polymer degradation, organogels, PDMS

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## Development of novel environmentally-friendly photoresists for use in the semiconductor industry

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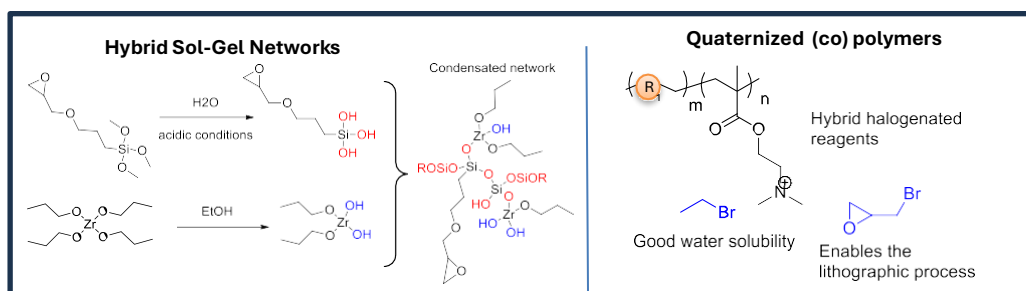
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Lithographic technology plays a critical role in semiconductor manufacturing, enabling the precise patterning of integrated circuits with reduced dimensions. However, traditional photoresist formulations usually rely on highly toxic and environmentally harmful solvents and chemicals [1]. Our approach aims to address this problem by developing new material platforms that can be processed in water or other 'green' solvents, while being compatible with the 'state of the art' lithographic exposure tools (Deep UV, e-beam and EUV) and maintaining the efficiency standards of the semiconductor industry.

In this context, hybrid materials containing silicon alkoxides, which allow the incorporation of metals such as Zr and Hf, were designed and investigated by exploiting a sol-gel chemistry route. Furthermore, random (co)polymers were synthesized and modified via a quaternization reaction to introduce the required material properties, such as stiffness, solubility and high etch resistance. In both cases, chemical amplification was employed by an acid catalyzed cross-linking reaction of the epoxy rings after irradiation [2]. Our results demonstrate a successful negative tone lithographic process at 248 nm with contrast curves and patterns which upon optimization highlight the potential use of the materials in environmentally friendly high-resolution lithography.

**Keywords:** Lithography, green hybrid materials, sol-gel chemistry, quaternization



**Figure 1.** Schematic representation of the two materials employed in the development of the green resists

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## GelMA-based hydrogels as scaffolds for lung cancer cell cultures

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Cancer is one of the common causes of death worldwide and a major public health problem. A recent study reported 10 million cancer deaths globally, while lung cancer was identified as the leading cause of cancer-related deaths [1]. Cancerous tissues exhibit unique biophysical characteristics that differentiate them from those of healthy tissues. During tumorigenesis, the extracellular matrix (ECM) undergoes remodeling followed by changes of its biomechanical properties, such as stiffness, causing abnormal regulations to cellular functions [2]. Biomaterial hydrogels, have been employed as *in vitro* models to reproduce these complex conditions of the ECM [3]. However, an in-depth study of malignant cell-ECM interactions and cellular dysfunctions is hindered by conventional hydrogel scaffolds and more advanced and responsive systems are required.

Herein, we report the successful synthesis of hydrogel scaffolds comprising gelatin methacrylamide (GelMA) and dopamine methacrylamide (DMA), in the form of thin films, *via* a photo-polymerization reaction. Specifically, scaffolds of different cross-link densities were prepared and characterized in terms of their rheological and swelling properties. A higher degree of functionalization of GelMA and a higher initiator concentration resulted in stiffer hydrogels with higher moduli and lower swelling ratios. Additionally, significantly higher moduli were measured for the GelMA-co-DMA hydrogels, indicating a higher cross-link density due to the additional cross-links formed by the catechol-catechol physical interactions among the DMA moieties. Our results demonstrate that adjusting key synthetic parameters, allows the fabrication of hydrogel scaffolds with tunable stiffness in order to more closely reproduce the ECM remodeling.

The prepared hydrogels were employed in *in vitro* cell studies using lung cancer cells and exhibited excellent cell attachment and viability. These hydrogels were further used to simulate the complex mechanical and hypoxic conditions of the pathological tissues, aiming to understand the growth of cells and their response to therapies in the tumor microenvironment.

**Keywords:** lung cancer, scaffolds, hydrogel, stiffness, hypoxia

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## Topological Mixtures Based on Ring Polymers: Linear Viscoelasticity

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The rheology of ring polymers is markedly different from the one of their linear counterparts due to the absence of free ends. Most notably, systematic experiments with carefully characterized ring polymers having molar masses above the entanglement limit for linear chains, show a power-law stress relaxation without an entanglement plateau and a much weaker molar mass dependence of the zero-shear viscosity compared to their linear precursors. By blending ring polymers with linear or branched macromolecules, rings experience threading, that leads to significant changes in their relaxation dynamics, and is described by constraint release (CR). In this work, we investigate the linear viscoelastic properties of a series of ring-containing blends, including both symmetric and asymmetric ring-linear mixtures, as well as ring- branched polymer systems. We report a pronounced non-monotonic dependence of blend viscosity in composition, strongly affected by the molar mass, the asymmetry, polymeric architecture and chain flexibility. These results highlight the critical role of entropic interactions and topological constraints in blend dynamics. Aiming to understand more the nature of threading mechanism, we compare the experimental data with a CR-based model of ring-linear blends which predicts the stress relaxation function in the low fraction regime of the ring component. This study aims to contribute to a deeper understanding of threading phenomena and their consequences on the macroscopic response of topological blends, suggesting ways to entropically tailor the properties of polymeric materials.



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## Novel PEDOT-based Blends for Electronic Skin Applications

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The development of multi-functional electronically active materials which mimic the properties of biological skin (electronic skin) has recently drawn significant scientific attention, mainly driven by their long-awaited incorporation in robotic systems and biomedical applications.

In this work we report on the development of novel polymeric materials that concurrently exhibit electronic conductivity, stretchability and the ability to self-heal, designed to be used in electronic skin applications. We opted to work with blends of a conductive and an insulating polymer, each contributing its own merits. Specifically, the conductive poly(3,4-ethylenedioxythiophene) doped with polystyrene sulfonate (PEDOT:PSS) was chosen, due to its high electrical conductivity, in combination with polyurea (PUR), an amorphous polymer which provides the final blend with the desirable mechanical and self-healing properties.

A series of PUR/PEDOT:PSS blends with varying weight fractions was prepared in an effort to find the ideal balance between conductivity and mechanical properties, and the effect of composition on the performance of these blends was evaluated. Electronic conductivity was characterized through four-point probe measurements and it was found that all blends possess higher conductivity than the neat PEDOT:PSS. To understand these results, UV-Vis absorption and x-ray photoelectron spectroscopy (XPS) measurements were performed to derive information about the doping level of PEDOT:PSS. The structure of the blends was characterized by atomic force microscopy (AFM) and grazing incidence wide-angle x-ray scattering (GIWAXS). The materials stretchability was evaluated through extension tests and the self-healing ability through optical microscopy. After self-healing, conductivity and mechanical properties were re-measured in order to evaluate the samples recovery and the reproducibility of functional properties upon self-healing.

**Keywords:** E-skin, Conducting Polymers, PEDOT:PSS, Blends, Self-healing

**Acknowledgements:** This research is carried out within the framework of the National Recovery and Resilience Plan "Greece 2.0", funded by the European Union – NextGenerationEU (Implementation body: HFRI, project ID: 16618)



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## Mechanochemical Recycling of Polyacylhydrazones via Selective Bond Cleavage in Aqueous Media

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Recent advances in polymer mechanochemistry have demonstrated how mechanophores—molecular motifs engineered for selective bond cleavage under mechanical stress—enable precise control over material degradation [1].

Herein, we introduce water-soluble polyacylhydrazones, designed to degrade under low-frequency ultrasound. These amphiphilic polymers, synthesized from poly(ethylene glycol) and aromatic building blocks, undergo controlled scission at 24 kHz, utilizing the acylhydrazone moiety's specific sensitivity to sonication, offering a sustainable path for polymer recycling [2-3]. We tracked the acylhydrazone bond cleavage using high-resolution <sup>1</sup>H NMR spectroscopy, while size-exclusion chromatography confirmed the selective main-chain fragmentation, indicated by a consistent decrease in molecular weight. The degradation process was further investigated by UV-Vis spectroscopy, providing insights into the response of these polymers to ultrasonic forces.

This system enables the effective polymer degradation under mild aqueous conditions and mimics commercial recycling processes, in which cavitation-driven shear forces selectively cleave the acylhydrazone bonds [4]. By substituting the energy-efficient ultrasound stimulus with conventional thermal or chemical treatment, we present a new approach for closed-loop recycling. The combination of water solubility and mechanical specificity in these polyacylhydrazones represents a breakthrough in designing future recyclable materials aligned with the green chemistry principles.

**Keywords:** mechanochemistry; polyacylhydrazones; main-chain polymer degradation; polymer recycling

**Acknowledgements:** The authors acknowledge funding by the “BIOPHILES” “Theodore Papazoglou” FORTH Synergy Grants 2024.

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## Investigation of Crystallization Kinetics in Poly(ethylene oxide)-based Nanocomposites utilizing Simultaneous Small- and Wide-Angle X-ray Scattering

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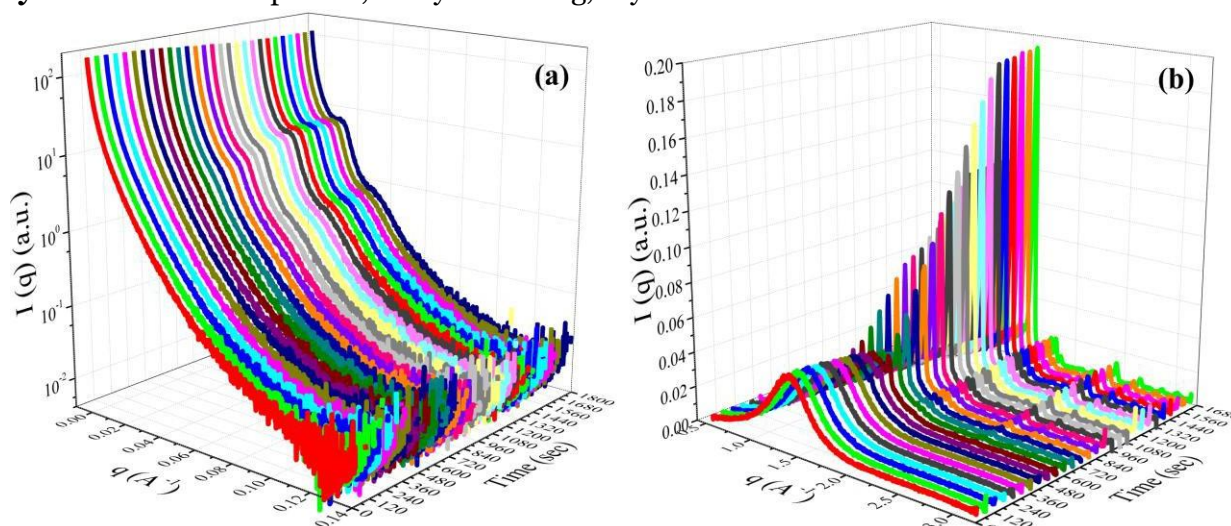
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It is well known that polymer morphology, dynamics, and properties can be significantly altered by the incorporation of nano-additives in the polymeric matrix, forming nanocomposite materials. Moreover, investigation of the crystallization behavior of semicrystalline polymers is of paramount importance since it largely determines their final properties. In this work, the effect of silica nanoparticles (SiO<sub>2</sub>) on the microstructure and crystallization kinetics of poly(ethylene oxide) (PEO) in PEO/SiO<sub>2</sub> nanohybrids is investigated using simultaneous Small- and Wide-Angle X-ray Scattering (SAXS/WAXS). Isothermal measurements were performed over a broad temperature range, and the influence of nanoparticle content was examined by synthesizing hybrids of varying composition. The results indicate that increasing the amount of nanoparticles leads to decreased crystallinity and smaller crystal long period. Additionally, SAXS measurements reveal the formation of a network structure even at low nanoparticle concentrations. These structural changes are attributed to enhanced interactions between PEO and SiO<sub>2</sub>, resulting in a more organized morphology, as confirmed by rheological data as well [1]. Overall, this study highlights the importance of nanoparticle concentration in tuning the properties of polymer nanocomposites something important in their utilization in advanced applications.

**Keywords:** Nanocomposites, X-ray Scattering, Crystallization kinetics



**Figure 1.** Isothermal (a) SAXS and (b) WAXS measurement of PEO at 50 °C.

**Acknowledgements:** This work was supported by the EU Horizon Europe Programme (project WISE, Grant Agreement 101138718).

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## Effect of Graphene Derivatives on the Self-Healing Efficiency of Polyurethane Nanocomposites

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Self-healing coatings have attracted growing research interest due to their ability to autonomously repair damage caused by external forces [1]. Polymeric materials, and more specifically polyurethanes, comprise one of the most promising materials to use towards this direction [2]. Furthermore, the development of polymer nanocomposites based on the incorporation of nano-additives within a polymeric matrix is a widely used strategy to enhance their mechanical, thermal and self-healing properties [3].

In this study, graphene oxide (GO) was synthesized via a modified Hummers' method from graphite and was subsequently reduced using hydroiodic acid (HI) to obtain reduced graphene oxide (rGO). Additionally, partially reduced graphene oxide (p-rGO) was synthesized by adjusting the amount of reducing agent. These graphene derivatives were incorporated in different amounts into a waterborne polyurethane dispersion based on a polycarbonate polyol to develop nanocomposites with different composition and to investigate their effect on the self-healing properties.

The self-healing ability of the pure polyurethane was found to be enhanced in the nanocomposites and the healing rate was found much higher, due to either better heat dissipation and/or the enhanced ability for hydrogen bond formation. The effect of the nanohybrid composition, the degree of reduction as well as of the different concentration of oxygen groups were evaluated in order to determine the mechanisms responsible for the observed improvement in the self-healing performance.

**Keywords:** Self-healing coatings, polyurethanes, graphene derivatives

### Acknowledgements

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## Shear-Induced Microstructural Evolution in Depletion Colloidal Gels: The Role of Attraction Range

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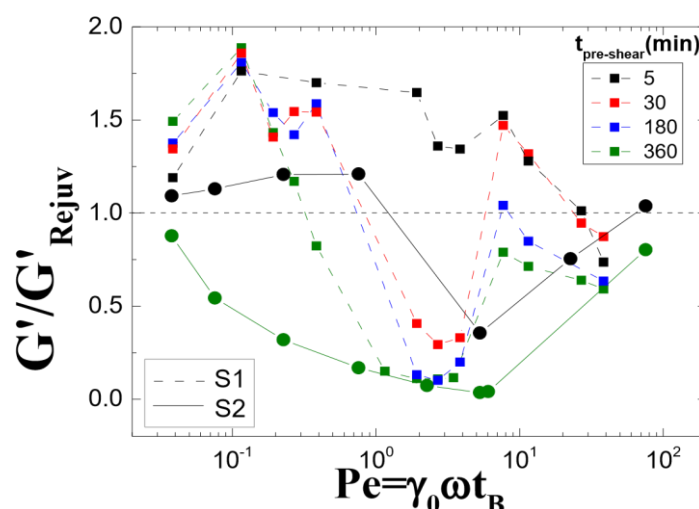
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In this study, we investigate the shear-induced microstructural changes in intermediate volume fraction ( $\phi=0.44$ ) colloid-polymer gels. We used a suspension of hard-sphere colloidal particles with a short-range depletion attraction, induced by adding non-adsorbing linear polymers. More specifically, the addition of the non-adsorbing polymer generates a tunable attractive interaction between the colloids. In our depletion system composed of sterically stabilized PMMA particles and non-adsorbing polymers, we will probe the structure of the gel for different depletion interactions.

This technique allows us to directly image the 3D structure of the colloidal gel and track how the particle arrangement changes across different parameters — especially the polymer concentration, which controls the range and strength of the depletion attraction. We vary the range of attraction by using different hard spheres (HS) particle radius and PB molecular weight, corresponding to polymer-to-colloid size ratios of approximately 0.02 and 0.2. We investigate the use of a specific shearing protocol based on steady and oscillatory shear [1], to identify the most efficient pre-shear protocols for controlling the gel strength and its flow behaviour, i.e. for tuning its linear viscoelastic moduli and its yield strain and stress. Both steady and oscillatory shear protocols are therefore explored to gain a comprehensive understanding of the gel structural evolution and its corresponding mechanical response. Interestingly, we observe that increasing the attraction range, (keeping the same attraction strength) leads to a decrease in the elastic modulus  $G'$ , and we use confocal microscopy to probe any related microscopic structural changes.

**Keywords:** colloid-polymer mixtures, depletion interaction, colloidal gels, shear induced control



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## Colloidal Dopants as Defect Mediators: Hybrid Particle-Field Simulations of Defect Control in Lamellar Block Copolymers

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Block copolymers (BCPs) are foundational to self-assembled nanostructured materials, offering precise control over nanoscale morphology through microphase separation. Yet, topological defects are inherent to these systems. While historically considered undesirable in material design, emerging strategies now exploit defects as intentional design features in nanolithography, enabling the templating of non-periodic nanostructures for advanced electronics[1].

Our work employs hybrid field- and particle-based simulations to investigate how dopant colloidal particles mediate energy landscape modifications that govern defect formation and stabilization in lamellar BCPs. We address two unresolved questions: (1) how molecular-scale dopant-defect interactions propagate to mesoscale topological features, and (2) whether kinetic pathways can be deliberately manipulated to access defect configurations inaccessible at equilibrium. Furthermore, we propose that stimuli-responsive dopants, which can react to temperature, light, or chemical cues, could enable the dynamic reconfiguration of defect architectures.

**Keywords:** block copolymer, topological defect, colloidal particles, field simulations

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## Molecular Dynamics Study on the Formation and Mechanical Properties of Polymer-Grafted Nanoparticle Films

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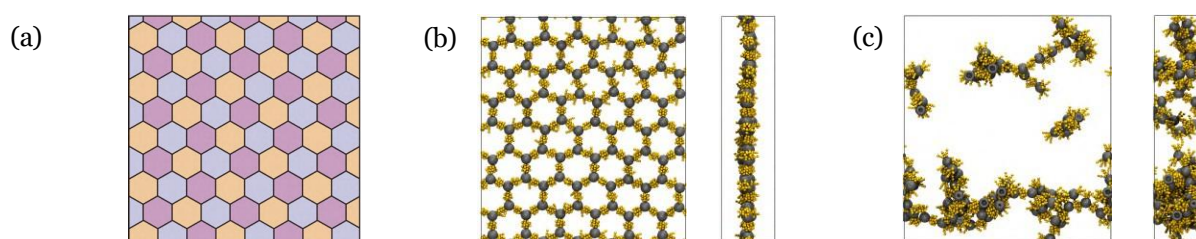
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Polymer nanofilms, with their self-supporting, quasi-two-dimensional structure and controlled nanoscale thickness, have attracted significant interest for applications in optical devices, thin-film batteries, coatings, and adhesives. The self-assembled structures in their nanocomposites are closely linked to their physical properties and functionality. A promising approach for controlling these structures is the introduction of polymer-grafted nanoparticles [1], which form highly directional interactions to create physical "bonds". By adjusting parameters such as polymer type, chain length, graft density, and graft position, various morphologies can be achieved. In polymer systems, recent studies have shown that certain Archimedean tiling patterns can be reproduced using three-component star-shaped polymers [2]. This study focuses on the formation of free-standing superlattice nanofilms with Archimedean tiling structures through the self-assembly of polymer-grafted nanoparticles. Molecular dynamics simulations are used to identify key structural parameters—such as graft density, chain length, and chain stiffness—that enable the formation of the desired Archimedean tiling structure. Additionally, uniaxial tensile simulations are performed to examine the relationship between structural and mechanical properties. These properties are critical for evaluating the films' mechanical performance in real-world applications. Tensile strength reflects a material's ability to withstand stress, while relaxation time provides insight into its flexibility and viscoelastic behavior.

**Keywords:** polymer nanofilm, molecular dynamics, self-assembly, Archimedean tiling



**Figure 1.** (a) Target honeycomb-type Archimedean tiling and its self-assembly outcomes: (b) successful and (c) failed.

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## PAINTing the nanoscale heterogeneities in supramolecular solvated networks

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Low Molecular Weight Gelators (LMWGs) are small molecules that self-assemble into onedimensional nanofibers. These can entangle to form three-dimensional networks that immobilize solvents and form supramolecular gels.<sup>1</sup> Characterizing the dynamic behaviour and sensitivity to external conditions of these gels in their native solvated state is challenging. In this scope, Point Accumulation in Nanoscale Topography (PAINT), a single molecule fluorescence imaging technique, could unveil their structures and dynamics previously unattainable because of the optical diffraction limit in classic microscopy. This technique affords nanometric resolution like Electron Microscopy (EM) and Atomic Force Microscopy (AFM), but in addition allows for targeted contrast enhancement and room-temperature dynamics in solvated samples.<sup>2</sup>

PAINT operates on the premise of detecting transient non-specific or specific physisorption of single fluorophores onto the object of interest.<sup>3</sup> In this work environment sensitive push-pull chromophores, such as Nile Red<sup>4</sup>, featuring electron-donating and electron-withdrawing groups, are employed for tag free imaging of the supramolecular peptide-based hydrogels. With this approach simultaneous super resolution visualization of the self-assembled networks and probing of the local gel microenvironment can be achieved.

In particular, nanoscale heterogeneities are highlighted at the single molecular level by means of timetrace recordings of binding events over relevant super-resolved architectures, such as nodes and fibers. The quantified binding affinity and fluorescence intensity variations, demonstrate a gelator concentration dependence of the hydrophobicity of the respective binding pockets, responsible for the overall evolution of the network morphology along the concentration gradient. Combining PAINT microscopy with environment sensitive fluorescent probes, highlights the potential of this technique to uncover useful information concerning the hydrogel self-assembling properties and helps shine light to understand parts of soft matter that previously remained in the dark.

**Keywords:** nanofibers, self-assembly, low molecular-weight gelators, fluorescence microscopy, super-resolution

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## Self-Assembled Hierarchical Membranes of Hyaluronic Acid and Amphiphilic Peptides

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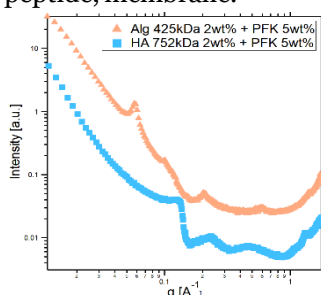
Self-assembled membranes formed at the interface between two oppositely charged aqueous solutions of polyelectrolytes and self-assembled peptides were first reported when negatively charged Hyaluronic acid (HA) was brought into contact with a positively charged peptide-amphiphile (PA) (C<sub>16</sub>V<sub>3</sub>A<sub>3</sub>K<sub>3</sub>) [1]. These membranes exhibited a hierarchical structure of three distinct areas, including a region of perpendicular fibers, which was found to be essential for the membrane's stability.

We recently reported on the formation of similar membranes at the interface of a cationic  $\beta$ -sheet peptide PK(FK)<sub>5</sub>P (PFK) aqueous solution and a negatively charged aqueous alginate solution. Utilizing SAXS and SEM, we found that these membranes can form the expected three-region structure, including perpendicular fibers; but can also form a stable structure of a single amorphous region lacking these standing fibers. Based on these results, we identified critical parameters affecting the reaction-diffusion process taking place at the interface and the growth of perpendicular fibers. We suggested a modified mechanism for these membranes and were able to control their structure and mechanical properties [2].

Substituting alginate with other polysaccharides revealed that the polymer chain and ensemble characteristics play an important role in determining the resulting membrane features [3]. Moreover, creating HA/PFK membranes has been proven to be a more challenging task than originally anticipated, as precipitates were formed over a wide range of assembly conditions.

Here, we aim to further our understanding of these self-assembled membranes by utilizing SAXS and SEM to investigate parameters that can affect their hierarchical structure (e.g., HA Mw, the identity of the peptide's charged amino acid, etc'), as well as the initial interactions between PFK, PA and HA. Our findings indicate that the peptides exhibit distinct characteristics, such as variations in assembly rate and surface charge, both of which significantly influence their initial interactions with the HA, thus affecting the membrane formation mechanism.

**Keywords:** self-assembly, amphiphilic-peptide, membrane.



**Figure 1.** Small angle X-ray scattering (SAXS) 1D curves of membranes made with 5wt% PFK and alginate solution (▲) or HA solution (■). The curves show differences in the nanostructures of the membranes.

**Acknowledgments:** This work is supported by the Israel Science Foundation ISF 673/23

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## The Existence and Formation Dynamics of Supramolecular Chains in Equilibrated and Sheared Ring Polymer Melts

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Despite significant advances in polymer physics, the entanglement mechanisms between ring polymers remain largely unexplored. This study investigates the existence and formation dynamics of deadlocks - temporary topological constraints that can form between rings - in melts of nonconcatenated and unknotted rings under both equilibrium and steady-state shear conditions. To enable this investigation, we enhanced an existing topology-based deadlock detection algorithm [2], allowing for a more detailed classification of the deadlocked state by defining a new statistical quantity: the degree of deadlocking.

Under equilibrium conditions, we find that deadlocks are a natural feature of the ring polymer melt, with a population of deadlocked pairs constituting approximately 1% of all linearly non-separable pairs. Among these, only 5% exhibit a strong deadlocked state. The degree of deadlocking is strongly correlated with the persistence of deadlocked pairs: those with a low degree disentangle rapidly, while those with a high degree exhibit meta-stability, persisting for several diffusion times. Under steady-state shear conditions, our findings show that the population of deadlocks is significantly higher compared to equilibrium, with pairs exhibiting a high degree of deadlocking being more than 15 times as frequent. We observe two distinct regimes for the degree of deadlocking: pairs with a low degree disentangle rapidly whereas pairs with a high degree *can* persist for longer times and their formation frequency is periodic, potentially related to the tumbling dynamics of the rings.

We devised a method to detect and classify entanglements in rings and showed them being relevant in dynamical context in- and out- of equilibrium.

**Keywords :** Ring Polymer entanglement, Topology, Molecular Dynamics Simulations

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## Synergistic Effects in PVOH-Pluronic Systems: A Study on Rheology and Thermal Behavior

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PVOH and Pluronic are known to undergo sol-gel transition independently through hydrogen bonding, crystallization, or micellization, as extensively documented in the literature. However, their combined behaviour remains largely unexplored. By blending these polymers, it is possible to fine-tune the critical gelation temperature, offering potential applications in 3D printing, drug delivery, and water treatment. This study aims to bridge the knowledge gap by investigating the rheological and structural evolution of PVOH solution-Pluronic solution hybrid systems. Temperature sweep rheology, along with XPS and XRD, was used to analyse gelation behaviour. In PVOH solution, increasing Pluronic content (0–4 wt%, 15% total polymer) raised the sol-gel transition temperature ( $T_g$ ) by disrupting PVOH-PVOH interactions. At higher Pluronic concentrations (>25%), a second transition occurred at higher temperature due to dominance of micellar assembly. Power-law analysis revealed an increase in the exponent ( $n$ ) and a decrease in strength ( $S$ ) and fractal dimension, indicating a more liquid-like network with increased concentration of Pluronic. On the other hand, in Pluronic solution, increasing PVOH concentration reinforced hydrogen bonding, strengthening the gel network. This resulted in a lower  $n$ , higher fractal dimension, and increased gel strength. However, at elevated temperatures, reduced PEO solubility weakened PEO-PVOH interactions, accelerating the gel-to-sol transition. XRD and XPS confirmed that higher Pluronic content reduced binding energy of the system, while increased PVOH enhanced structural integrity. This study provides new insights into how PVOH-Pluronic interactions govern thermal transitions and network dynamics, enabling precise control over gelation properties.

**Keywords:** hybrid system, gelation temperature, phase transitions.

**Acknowledgements:** Financial support from Indian institute of technology, Kanpur is gratefully acknowledged

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## Linking Microscopic Structure to Optical Properties in Soft Plasmonic Complexes

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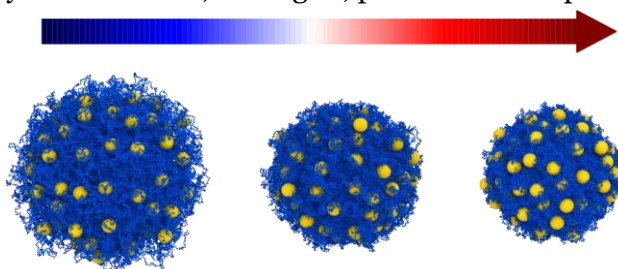
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Soft polymeric colloids such as thermoresponsive microgels have prompted significant advancements in soft matter physics as well as in nanotechnology. The possibility of tuning softness and temperature responsiveness by modifying the polymer network is not only ideal to investigate fundamental problems, but also offers the opportunity to design novel photonic materials through integration with plasmonic nanoparticles (NPs). This exploits the volume phase transition of microgels for tailoring the collective optical properties of NPs. Despite its great practical relevance, little attention was devoted to obtain a fundamental understanding of the microscopic details of NPs incorporation within soft colloids.

We fill this gap by combining Small Angle X-ray Scattering experiments and molecular dynamics simulations to study the temperature-dependent arrangement of gold NPs adsorbed onto microgels by means of electrostatic interactions. For the first time, we are able to connect the NPs spatial organization on the microgel with the optical properties of the complexes. We find that upon increasing temperature, NPs get closer due to microgel shrinking without forming clusters but they try to maximize their distance in order to reduce their mutual electrostatic repulsion. To unveil this behavior, we employ a simple model of NPs arranged on a spherical shell, which semi-quantitatively describes the intricate structure factors of NPs embedded within the microgel corona. Thanks to this approach, we finally establish the relationship between the degree of plasmon coupling and NP-NP distance, offering a pivotal step towards a precise control of the optical response of soft plasmonic complexes [1, 2].

**Keywords:** soft polymeric colloids, microgels, plasmonic nanoparticles



**Figure 1.** Simulation snapshots showing the thermoresponsive behavior of the microgel-NPs complex crossing the volume phase transition

**Acknowledgements:** Financial support by INAIL, Project BRIC 2022 ID 16 MICROMET is gratefully acknowledged.

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P. 155

# Mechanophore Crosslinking Effects in Nominally Brittle Hydrogels

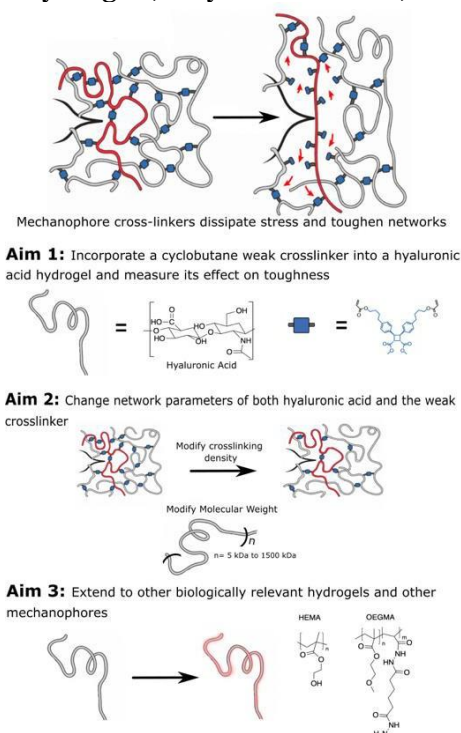
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The high water content and deformability of hydrogels make them well-suited to tissue engineering and drug delivery applications; however, hydrogels can be brittle and prone to mechanical wear. Recent work has found that the introduction of scissile cyclobutane-based mechanophore cross-linkers, which react via a facile force-triggered cycloreversion, leads to networks that are up to 9 times tougher than otherwise indistinguishable conventionally cross-linked analogs [1]. This improvement makes the materials less prone to fracture and wear without changing their performance in applications. This project is to see how the mechanophore effect can be applied to improving the toughness of biologically relevant hydrogels, such as those based on hyaluronic acid. In the long term, such material platforms might allow the influence of local fracture and tearing on the fate of cells embedded within them to be probed.

**Keywords:** Biologically relevant hydrogels, Polymer networks, Mechanophores



**Figure 1.** How weak bond mechanophores can dissipate stress to create stronger materials and the aims to modify them to work with hydrogels.

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## Protein-polysaccharide Complexes for Enhanced Food Supplement Delivery

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Polysaccharide-protein complexes are increasingly explored as delivery systems in biomedicine, pharmaceuticals, and food technology due to their safety, biocompatibility, and biodegradability. These systems are particularly valuable for encapsulating hydrophobic bioactive compounds, such as vitamin D<sub>3</sub> (VD<sub>3</sub>), to enhance their bioavailability, stability, and effectiveness. In this study, nanogels were formed through the electrostatic coassembly of  $\kappa$ -carrageenan ( $\kappa$ -CAR) and  $\lambda$ -carrageenan ( $\lambda$ -CAR) with bovine serum albumin (BSA) serving as a macro-ionic crosslinking agent. The distinct linear charge density and physicochemical properties of  $\kappa$ -CAR and  $\lambda$ -CAR enabled the formation of nanogels with varying structural characteristics. A combination of scattering techniques (light scattering, SAXS, SANS) and spectroscopic methods (FTIR, CD, fluorimetry) was used to investigate the microstructure of unloaded and VD<sub>3</sub>-loaded nanogels under different pH and temperature conditions.

Small-angle X-ray and neutron scattering revealed that complexes predominantly formed when BSA and carrageenan were mixed at acidic pH, with the protein serving as the major structural component. Notably, VD<sub>3</sub> addition enhanced complexation and stabilized nanogels above BSA's isoelectric point. Both carrageenans formed solvent-swollen structures, with  $\kappa$ -CAR generating larger, elongated aggregates and  $\lambda$ -CAR producing smaller, flat aggregates.

Fluorescence quenching, in combination with FTIR and CD spectroscopy, demonstrated the effective encapsulation of VD<sub>3</sub> within the nanogels. Spectroscopic analyses further revealed changes in BSA's secondary structure under varying environmental conditions.

This study highlights the value of combining scattering and spectroscopic techniques to achieve a comprehensive understanding of polysaccharide-protein-based nanocarriers. The findings underscore the potential of  $\kappa$ -CAR and  $\lambda$ -CAR nanogels as effective carriers for hydrophobic bioactive ingredients, offering promising applications in food engineering and nutraceutical development.

**Keywords:** carrageenan, BSA, polysaccharide-protein complex, VD<sub>3</sub> encapsulation, SANS, contrast matching



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## Standardized DNA Hydrogel Assembly for Programmable Delivery of Therapeutic Cargoes

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Hydrogels have a wide range biomedical and biotechnological applications according to their variable structural, rheological, and biological properties. The major challenges with current hydrogel formulations are that (i) their rheological properties cannot be easily tuned, (ii) they have limited ranges of compatibility with different families of biological cargoes, and (iii) they perform poorly for sustained biomolecule release.

DNA is an ideal substrate from which to construct new materials for biological applications because it is biocompatible, biodegradable, highly programmable, and exhibits predictable sequence-specific binding. Although current DNA hydrogels have been successfully applied to biosensing, drug delivery, tissue engineering, and cell culture and capture, there still lacks one standardized system that enables rapid design, assembly, and functionalization of DNA hydrogels for this broad range of applications.

We are building and characterizing a library of standardized DNA components for rapid design and assembly of a new suit of DNA hydrogels with predictable properties including tunable rheology [1], programmable capture of a broad range of biomolecules, controlled hydrogel degradation in biological environments, and sustained release of therapeutic cargoes.

**Keywords:** DNA hydrogels, therapeutics delivery, intelligent biomaterials

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P. 158

## Mechanistic insights into elastomer frictional wear using damage reporting mechanophores

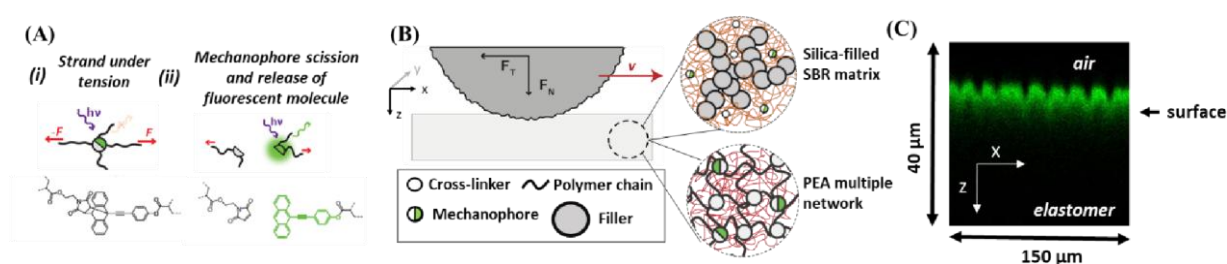
Ombeline Taisne<sup>1,2</sup>, Alex Cartier<sup>1</sup>, Côme Thillaye-du-Boullay<sup>1</sup>, Marc Couty<sup>2</sup>, Julien Caillard<sup>2</sup>, Costantino Creton<sup>1</sup>, Jean Comtet<sup>1</sup>

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Tire wear due to friction is a major issue for tire manufacturers. During wear by fatigue of tyre tread materials [1][2], the material at the surface of the tyre tread undergoes slippage at the road-tyre interface each time the wheel turns, leading ultimately to erosion through mass loss and wear. However, a mechanistic understanding of elastomer wear by fatigue is far from complete, due to the difficulty in accessing the local damage field at the surface of the material following mild frictional events.

Here, we take advantage of recently developed mechanophore molecules [3][4] to characterize molecular damage gradients in the sub-surface. Once chemically incorporated in known quantities in the elastomer network as cross-linkers, these molecules can be used to spatially probe molecular scission events damaging the integrity of the network (Fig. 1.A) [5]. Specifically, we use this detection strategy to characterize and quantify the damage gradient at a molecular scale in multiple interpenetrated networks elastomers made of poly (ethyl acrylate) (Fig. 1.B). Following mild friction cycles of the elastomer material against glass, we uncover that damage extends under the surface of the elastomer over tens of micrometers (Fig. 1.C). We further evidence a 2-step damage mechanism with a first regime showing spatially heterogeneous and non-linear accumulation of damage in the sub-surface of the material, followed by a regime of stationary damage, corresponding to the onset of material erosion. By varying the network architecture, we further demonstrate the occurrence of an intrinsic trade-off between fracture toughness and fatigue wear resistance in elastomers. Our experimental observations provide new insights to predict how accumulation of molecular damage leads to wear of soft materials.



**Figure 1:** (A) Mechanophore scission in the network probing chain-breaking events (B) Reciprocal sliding of a rough glass bead on the elastomer network, (C) Cross-sectional fluorescence image of the near surface region of a wear mark, reconstructed from a confocal microscopy scan.

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## Hybrid Pectin-Fibroin Microgels with Supramolecular cross-links and its Inter-linking

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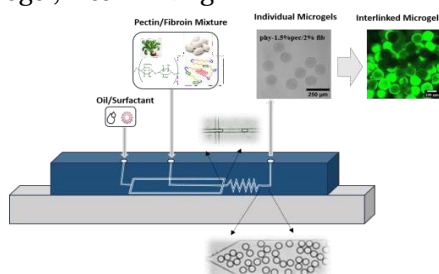
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Sugar beet pectin, a polysaccharide from industrial waste, and silk fibroin, a high molecular weight structural protein, can undergo gelation together via ionic interactions and conformational changes, leading to hydrogel formation. In this work, we have explored a microgel system based on pectin/fibroin combination and investigated its properties.<sup>1</sup> The pectin/fibroin microgels were fabricated using droplet-based microfluidics, and the secondary structure, mechanical properties, and degradation profiles were investigated. Our experimental results show that microgels exhibit an ordered  $\beta$ -sheet structure, Young's modulus in the range of 10 to 15 kPa, the degradation can be promoted using protease enzyme, and the bio-compatibility of the microgels is accessed using the Alamar blue cell viability assay with human pulmonary fibroblast (HPF). Furthermore, the microgels could be interlinked with each other via a chemical bonding or physical interaction, depending on the pectin/fibroin ratio, making it an ideal material for the highly porous scaffold that supports cell growth.<sup>2</sup> This research presents a highly functional hybrid biomaterial produced from waste products and a structural protein, demonstrating its cell compatibility and potential in tissue engineering applications.

**Keywords:** pectin, fibroin, microgel, inter-linking



**Figure 1.** Pectin/Fibroin microgel fabrication via microfluidics and the inter-linked microgel

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## Towards Sustainable Cleaning: Capillary Lifting Mechanism for Droplet Dewetting

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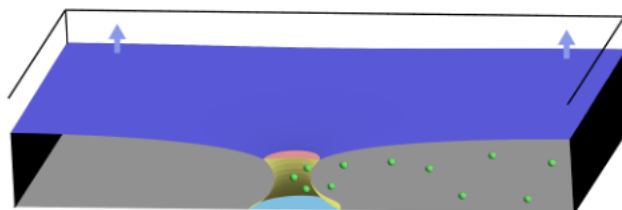
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Despite the pressing global water scarcity, both domestic and industrial cleaning processes heavily rely on vast quantities of water and the extensive use of surfactant. Here, we combine experiment and simulation to explore a droplet dewetting mechanism that minimizes resource usage (water, surfactants, and energy). Specifically, we induce the dewetting of an unwanted droplet from a surface using an immiscible working fluid. Experimentally, we designed a setup to manipulate the working fluid and observe the droplet evolution. Upon injecting the working fluid, the droplet forms a capillary bridge between the droplet-air and droplet-substrate interfaces (Fig. 1). As the working fluid rises, the bridge is stretched and eventually detached. Computationally, energy minimization methods [1] were used to systematically vary the interfacial properties, creating a dewetting prediction phase diagram and validating experimental observations. Our experimental and simulation results align regarding both the capillary geometry and dewetting outcomes, indicating the success of our model in facilitating the exploration of local droplet removal. Interestingly, our results show that considering a dynamic surface tension is crucial for working fluids containing chemicals, as interfacial tensions evolve differently at each interface. This work advances our understanding of fundamental ternary dewetting phenomena and demonstrates how interfacial properties can be leveraged to enhance cleaning efficiency while minimizing reliance on excess resources.

**Keywords:** Interfacial phenomena, Droplets, Wetting



**Figure 1.** An unwanted droplet being dewetting by an invading working fluid that contains chemicals.

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## Analysis of fracture processes in starch blended composites with a core-shell phase separated structure

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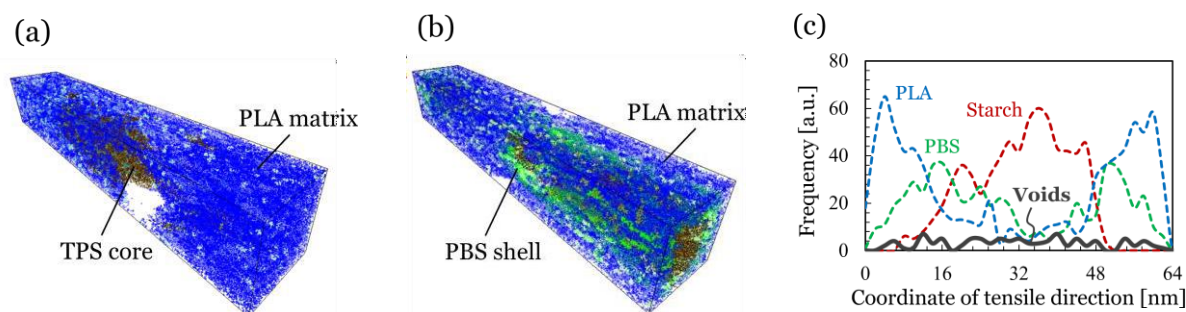
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The environmental impact of petroleum-derived plastics has become a critical concern due to increasing pollution issues. Polymer composites incorporating thermoplastic starch (TPS) have attracted attention as cost-effective and environmentally friendly biomass materials [1]. However, their low impact resistance remains a significant challenge, limiting their practical applications. In this study, we investigated the fracture processes of polylactic acid (PLA), polybutylene succinate (PBS), and TPS composites, which exhibit a self-assembled core-shell structure and enhanced impact strength [2], using all-atom molecular dynamics (MD) simulations.

To investigate the toughening mechanisms, we constructed two simulation models: a binary PLA/TPS model and a ternary PLA/PBS/TPS model. First, to enhance molecular diffusion and promote interfacial compatibilization between different molecular species, we performed structural equilibration simulations designed to replicate the melt-blending of plastic materials for each model. Subsequently, tensile deformation simulations were conducted to compare their fracture behaviors. The results showed that in the PLA/TPS model, the weak interfacial compatibility between PLA and TPS caused interfacial delamination (**Figure 1(a)**), leading to premature failure of the entire model. In contrast, in the PLA/PBS/TPS model, PBS infiltrated both the PLA and TPS phases, forming a thick compatibilized interfacial layer that effectively suppressed delamination (**Figure 1(b)**). Furthermore, in the PLA/PBS/TPS model, a moderate density of voids was observed to be uniformly distributed throughout the model (**Figure 1(c)**). These voids helped alleviate strain localization, thereby preventing abrupt failure and enhancing the overall toughness of the material.

These findings provide new insights into the fracture mechanisms of TPS-containing polymer composites and offer guidelines for designing high-performance biodegradable materials with improved mechanical properties.

**Keywords:** Thermoplastic starch, Molecular dynamics, Biomass polymer



**Figure 1.** Snapshots of (a) the PLA/TPS model and (b) the PLA/PBS/TPS model during the tensile simulation. (c) Voids and molecular distribution in the PLA/PBS/TPS model during tensile simulation.

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## Biohydrogen and Bioplastics Production from Organic Waste

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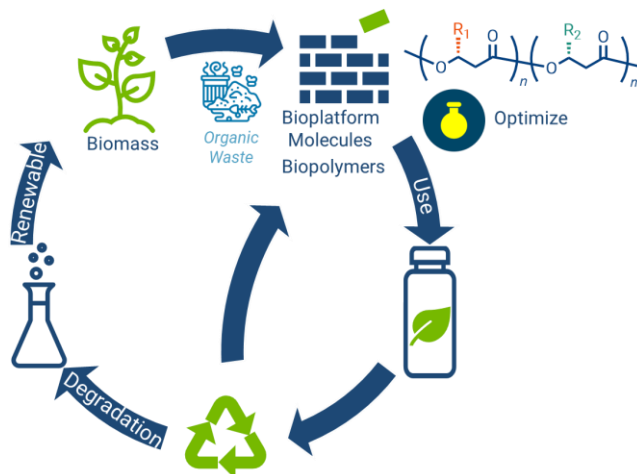
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A novel approach that converts biowaste into bioenergy (green production of hydrogen) and biopolymers (PHAs) in a balanced manner will be presented [1-2]. This approach aims to reduce the overall PHAs production cost on both a laboratory and a pilot plan scale, paving the way for its wider use in a plethora of applications. Dark fermentation was optimized to convert heterogeneous organic waste (including municipal organic waste and agro-industrial waste streams) to bio-hydrogen and volatile fatty acids (VFAs) [2]. The potential of the obtained VFAs to act as sole carbon source in various fermentation approaches was optimized for the synthesis of targeted -industrially relevant- PHAs [2]. Tailored PHAs (derivatives and blends with synthetic biodegradable polymers such as PCL, PLA and PVA) were also produced with the aim to improve performance and to offset the high price of PHAs.

**Keywords:** sustainability, bioplastics, circular economy



**Figure 1.** Schematic representation of the conversion of organic waste to bioenergy and bioplastics.

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## **Polyethylene and Polypropylene Take Different Routes to Micro/Nano-plastic Formation**

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In the environment, plastics are exposed to various aging factors that lead to the formation micro-nano plastics (MNPs). Polyethylene (PE) and polypropylene (PP) are the two most widely used polymers in the world. We investigate the mechanisms of fragmentation of these two polymers using a combination of chemical oxidation and mechanical stress. Although both are semicrystalline polymers, they respond differently to free radicals due to differences in their molecular structures.

Under quiescent oxidative degradation, both polymers undergo embrittlement, as confirmed by tensile testing. However, rheological analysis reveals that PE predominantly undergoes branching upon exposure to free radicals, leading to an increase in molecular weight and more solid-like behavior. In contrast, PP shows a tendency toward chain scission, primarily due to the presence of tertiary carbon atoms, which facilitate  $\beta$ -scission reactions. This results in a reduction in molecular weight and a more liquid-like rheological response.

We show that despite the differences in degradation mechanisms, both polymers exhibit brittleness and mechanical failure, ultimately leading to the release of micro- and nano-sized particles. To simulate environmental mechanical stresses, oxidized films were subjected to agitation at varying stirring speeds. A clear correlation was observed between the intensity of mechanical stress and the extent of MNP generation, with higher stirring speeds resulting in a greater release of particles.

Overall, we systematically demonstrate the deterioration of mechanical and rheological properties in both polymers due to chemical oxidation, as well as the subsequent formation of MNPs under mechanical forces. This work provides insights into the physicochemical pathways that drive polymer fragmentation in the environment.





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## **Cellulose based coatings from deep eutectic solvents: mechanical properties and topography**

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Cellulose is extracted on an industrial scale from wood derivatives via strong acid hydrolysis, a non green method. Alternatively cellulose nanocrystals (CNCs) can be extracted by utilizing deep eutectic solvents (DES). When dispersed in water the CNCs form gels at relatively low concentrations (compared to acid derived ones) due to charge induced attractions. We utilize DES derived CNCs to form films for coatings. We explore the effects of the CNC suspension attractions and the role of the preparation protocol on the film and specifically on the mechanical properties and the topography of the final film. To this end we utilize Atomic Force Microscopy and Extensional deformation test. We are also exploring strategies to increase the hydrophobicity of the surfaces. We aim to tailor the properties of these films to fit applications such as green antibacterial and antifouling coatings.

**Keywords:** Cellulose, films, coatings, eutectic solvents



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## Synergistic Effect of TiO<sub>2</sub> and SiO<sub>2</sub> Coatings on Radiative Cooling in Textiles: From Experimental and Theoretical Perspectives to 9th International Soft Matter Conference – Greece

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Global warming poses critical challenges to maintaining thermal comfort, particularly in the energy-intensive textile industry. This study investigates the application of radiative cooling techniques to enhance the cooling performance of fabrics by applying composite coatings of titanium dioxide (TiO<sub>2</sub>) and silicon dioxide (SiO<sub>2</sub>) nanoparticles, selected to improve both solar reflectivity and thermal emissivity, respectively. The surface of the fabric was functionalized using benzophenone and acrylic acid to assure strong adhesion of metal oxide nanoparticles via hydrogen bonding, while their optimal size was selected using theoretical calculations based on Mie scattering principles. Statistical analysis across multiple testing days revealed significant cooling effects, underscoring the reliability and efficiency of the nanoparticle coatings. Experimental results demonstrate that compared to uncoated fabrics, cotton fabrics treated with these nanoparticles achieve a temperature reduction of up to 6.9 °C in direct sunlight. The dual functionality of TiO<sub>2</sub> to reflect solar radiation and SiO<sub>2</sub> to emit thermal radiation within the atmospheric window contributed to enhanced cooling performance of the fabric. These findings highlight the potential of nanoparticle-enhanced textiles to provide sustainable, energy-efficient cooling solutions, reducing the dependence on conventional air conditioning and contributing to environmental sustainability, promising to revolutionize the textile industry, improving comfort in warmer climates, and supporting global energy conservation efforts.



**Figure 1:** Schematic illustration for the mechanism of radiative cooling

## Interplay between Crystallization and Crosslinking in Semicrystalline Polyester-Based Vitrimers

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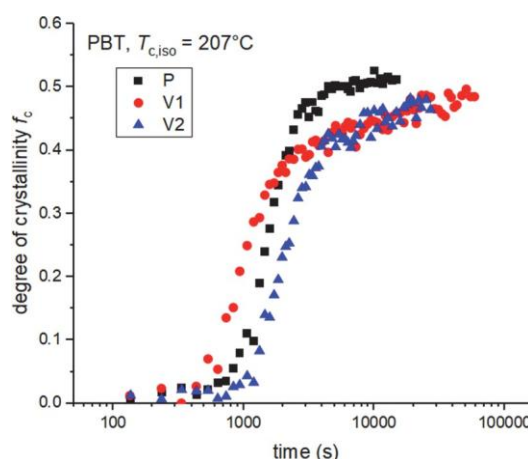
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Crosslinked polymers are intrinsically difficult to recycle. For this reason, vitrimers that feature dynamic covalent bonds and are thus able to flow and be reprocessed at elevated temperatures, have recently attracted significant attention. The concept has been conceived in the context of thermoset resins, but it also offers high potential at lower degrees of crosslinking. Ultimate properties of semicrystalline thermoplastic polymers in fact benefit from crosslinking, but again at the cost of a loss in processability. Also in this context, vitrimers with their ability to be injection-molded at elevated temperatures are under active discussion [1]. Yet, there are only few systematic investigations on the effect of (dynamic) crosslinking on the properties and morphology of semicrystalline polymers [2].

Here, we focus on a sustainable and application-relevant vitrimer system based upon poly(butylene terephthalate), PBT, harnessing the transesterification reaction at elevated temperatures. We have prepared and confirmed the favorable properties of such materials following previously published procedures [1]. We apply a combination of DSC, mechanical and rheological experiments for sample characterization and compare these findings with in-depth <sup>1</sup>H low-resolution NMR investigations of the crosslinking structure and the time-resolved crystallinity of the samples [2], following different thermal protocols. One focus of the work is the delicate balance between a necessarily low degree of crosslinking and the rheological properties of the melt on the one hand, and the semicrystalline morphology and ultimate properties of the final materials on the other hand. With this we hope to establish a systematic understanding of the property space of such materials.

**Keywords:** sustainable polymers, crystallinity, NMR spectroscopy, rheology



**Figure 1.** NMR-detected isothermal crystallization kinetics for differently crosslinked poly(butylene terephthalate)-based vitrimers (V1 and V2, resp.) vs. the pristine polymer (P). The crosslinking effect is clearly non-trivial.

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## Bi-functionalization of L-Lysine with aromatic and aliphatic moieties converts it into a Super Organogelator in DMSO

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Supramolecular gels are semisolid materials that have generated a lot of interest due to their distinctive characteristics and potential applications in various fields as soft materials.<sup>1</sup> These gels are formed from low molecular weight gelators (LMWGs), by self-assembling in organic or water-based solvents through intermolecular non covalent interactions, that entrap the liquid phase and create 3D network through capillary forces and surface tension.<sup>2–4</sup> The selfassembly nature of these LMWGs leads to various structures such as nanostrips, nanofibers nanostrands and often aggregates.<sup>5</sup> Organogels have been developed using various LMW organo-gelators in commonly used polar and non-polar solvents such as methanol, ethanol, benzene, toluene,<sup>8,9</sup> dichloromethane<sup>10</sup> and DMF.<sup>11</sup> These organogels have been extensively studied in a variety of domains, such as energy transfer and light harvesting<sup>12</sup>, cell imaging,<sup>13</sup> controlled drug delivery,<sup>14–16</sup> biomaterials,<sup>17,18</sup> and chirality. Additionally, organogels in rare solvents like silicon oils and 2-phenylethanol have been developed and reported as active antimicrobial agents. Furthermore, oil-based supramolecular organogels have been derived and used in pollution scavenging, as carriers for trans-dermal drug delivery, and in lubrication applications.<sup>19–20</sup> To the best of our knowledge, although several LMWG have been reported to form organogels in various organic solvents, reports of supramolecular gelation in neat DMSO remains scarce. DMSO is known for its strong hydrogen bond-disrupting ability, which often hinders the self-assembly processes required for gelation by LMWGs. Despite this challenge, a few notable examples of gelation in neat DMSO have been reported.

In the present work, we explore the tribological performance and oscillatory shear response of supramolecular self-assembled systems formed by the FmKPal gelator in organic solvent and base oil. Furthermore, blending the FmKPal DMSO gel with lubricant oil retains the gel behavior, highlighting its potential for oil-based applications. The current finding of DMSO gelation by an LMW gelator provides additional insights into supramolecular gel formation and offers a lead for designing similar gelators with broader applications, such as lubrication and related fields. Notably, the minimum gelation concentration (MGC) of FmKPal in DMSO is as low as 0.2wt%, which is significantly lower than the typical 1–2 wt% observed for most LMW organogelators. This exceptionally low MGC classifies FmKPal as a “super” organogelator.

**Keywords:** Amino acid:, LMW gelators, organogel, DMSO

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