10TH INTERNATIONAL SOFT MATTER CONFERENCE (ISMC 2026)

Oral Presentations

(Plenary)

Soft matter under heterogeneous deformation: stretching, alignment, and instability

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Soft materials in flow experience nonuniform deformation fields in which shear and extension coexist, often under different boundary conditions. Although confined microfluidic flows and free-surface filament stretching differ in geometry and interfacial constraints, they share a common response: flow-induced microstructural deformation, alignment, and relaxation in complex fluids (from polymer solutions to colloidal suspensions). In this talk, I will show how these responses under heterogeneous shear–extensional deformation provide a unifying lens for fluid–structure interactions, viscoelastic instabilities in microfluidics, and filament dynamics in 3D printing.

I will first discuss how extensibility controls flow-induced alignment across flexible polymers and rod-like colloids, linking microscopic stretching dynamics to macroscopic ordering. I will then turn to confined geometries—micropost arrays and porous media—where localized extensional hot spots embedded in shear-dominated flows can trigger viscoelastic instabilities and strong coupling to boundaries. Finally, I will connect these mechanisms to free-surface flows in direct ink writing, where extrusion transitions from shear-dominated flow in the nozzle to extension-dominated filament formation. By decoupling shear rheology from extensional response, we identify a timescale-based criterion that predicts filament stability, turning printing from trial-and-error into a predictive soft-matter design problem.

Some inverse problems in soft and active matter

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How can one grow a face or a flower from a flat sheet? Fold a sheet into an origami pattern? Control phase separation? Transport a drop of active matter? Steer an ant swarm? Heal a wound? I will discuss potential answers to some of these inverse problems that unites ideas from optimal control and optimal transport for the steering of particles and fields.

Rheological Universal Differential Equations:

Scientific Machine Learning the genetic fingerprint (or *Rhe-ome*) of complex fluids

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The formulation of tensorial rheological constitutive equations relating internal stresses and deformations in complex fluids is a critical step in the engineering of soft material systems. While data-driven models provide accessible alternatives to expensive first principles models and less accurate empirical models in many engineering disciplines, the development of similar models for complex fluids has lagged. The diversity of techniques for characterizing non-Newtonian materials and complex flows creates a challenge for classical machine learning approaches, which require uniformly structured training data. Consequently, early machine-learning based constitutive equations have not been portable between different deformation protocols or mechanical observables, and in many cases are not frame-invariant or capable of predicting phenomena such as the development of large normal stress differences. Here, we present a data-driven framework that resolves such issues, allowing rheologists to systematically construct learnable models that incorporate essential physical information [1]. Our framework incorporates a universal approximator within a materially objective tensorial constitutive framework. By construction, the resulting *Rheological Universal Differential Equation* (RUDE) respects physical constraints, such as frame-invariance and tensor symmetry, required by continuum mechanics. Proper dimensionless scaling of the RUDE and the implementation of concepts from curriculum learning enable the incorporation of progressively more complex rheometric test data over a wide range of dynamic scales. We demonstrate that the resulting framework facilitates the rapid discovery of accurate constitutive equations from limited data and that the learned models may then be used to describe more kinematically complex flows. This inherent flexibility enables the application of these “digital fluid twins” to a range of material systems and engineering problems.

We demonstrate that multimode formulations of the universal differential equation may be trained on a variety of data (e.g. steady shear flow, SAOS and LAOS shearing deformations as well as more complex kinematic histories) and then applied to predict fluid properties in a multidimensional simulation of an industrially relevant flow. Once learned, the RUDE encodes the full rheological response of a complex fluid or soft solid material and may thus be envisioned as a digital portrait encoding the *rhe-ome* of the material. At the heart of this *rhe-ome*, the linear viscoelastic response is captured in a classical set of discrete relaxation times and moduli, which thus constitute the fundamental ‘base pairs’ of the material. Using the theory of matrix polynomials pioneered by Rivlin and Spencer in the 1950s, the complete nonlinear response is captured by eight frame-invariant tensor products; which may thus be visualized as the ‘chromosomes’ (or, perhaps, the *rheosomes?)* that capture the full range of rheological responses of a material in any deformation history. Once learning is complete, the functions formed from the scalar invariants of these eight tensor products – and the relative weights of the universal differential approximator – represent the effective proteomic outputs expressed for a particular complex fluid in a specific flow history. This framework provides a useful visual metaphor as well as a powerful mechanism for assimilating material-specific data into a single company-wide or community-wide database and opens broad avenues for future soft material design and process engineering.

[1] Lennon, K.R., McKinley, G.H., Swan, J.S., *Proc. Nat Acad. Sci.* (2023), **120** (27) e2304669120.

In silico microgels

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Colloidal microgels are a favourable model system in experiments due to their softness and responsiveness, as well as theoretically as the prototypes of soft colloids.

In recent years, we established an in silico method able to realize numerical microgels with unprecedented similarities to experimental ones. In this talk I will review the main results of this approach at the level of single particle or of an ensemble of microgels and finally discuss the important of microgel internal architecture on the collective properties of dense suspensions.

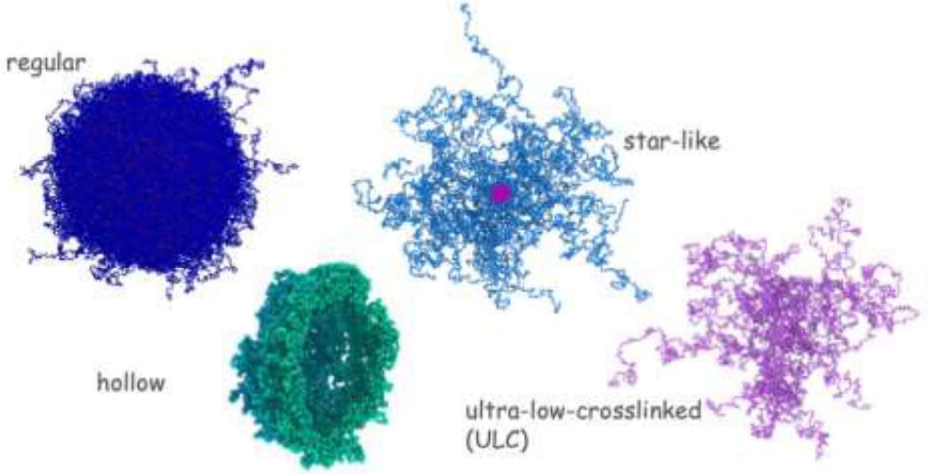

Fig.1 Snapshots of different types of in silico microgels

Tunable Matter

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In 1972 Phil Andersen articulated the motto of condensed matter physics as “More is different.” However, for most condensed matter systems, the behavior of many more constituents is quite similar to that of more. Here I argue for a class of condensed matter, “tunable matter," in which many more is more different—the behaviors of more and of many more can be quite different. A familiar example of tunable matter is the brain, whose cognitive capabilities increase as size increases from 302 neurons (C. Elegans) to a million neurons (honeybees) to 100 billion neurons (humans). I propose that tunable matter provides a unifying conceptual framework for understanding emergent collective function in a wide class of biological systems, and motivates new non-biological systems capable of being trained to develop desired complex collective behaviors without using a processor.

Renewable Living Matter - anomalous elasticity, force patterning and excitability

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Living systems offer a fundamentally different perspective on functional, adaptive materials. One need only consider their capacity for self-healing, regeneration, and inheritance to be persuaded by this viewpoint. Unlike conventional engineering materials, where rigidity arises from internal architectures at equilibrium and is set by a stable energy minimum, living materials operate far from equilibrium. Maintained by internal forcing and environmental feedback, they generate rigidity through self-assembly rather than inheriting it from a pre-designed architecture. At the heart of this is material renewability and mechanical adaptation, prototypical examples include the cellular cytoskeleton and the epithelial tissue.

In this talk, I will present a continuum hydrodynamic description of the renewable actomyosin cytoskeleton: where active constituents generate and sense contractile forces, whose interplay with soft elastic modes drives it toward marginally stable states. Instead of collapse, these soft modes self-organize stress (and material density) into evolving networks of lower-dimensional force-bearing structures—force chains and force sheets —which sustain the applied load while remaining highly reconfigurable. Further, the nonreciprocal interplay between active stresses and renewability, drive sustained excitability, giving rise to travelling waves and pulses in this purely mechanical system. Rather than asking for prescribed material properties, our work advocates treating living materials as having dynamically evolving rigidities facilitated by adaptive turnover, leading to various functional phenotypes.

Ciliary fluid dynamics of swimming, feeding, pumping, and sensing

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Cilia are cell organelles acquired by eukaryotes more than a billion years ago that induce flow in the surrounding fluid by periodically beating in waves [1]. Many eukaryotes, from microorganisms to humans, possess cilia. From the viewpoint of biofluid mechanics, cilia perform four major functions: swimming, feeding, pumping, and sensing.

In this article, we explain the flow produced by cilia and its biological functions. First, the swimming speed and efficiency of ciliary swimming are discussed [2]. It is shown that the friction between cilia and the cell surface is extremely large. Our analysis reveals that swimming efficiency is highest when the number of cilia increases in proportion to the square of the body length. The relationship of microorganisms in nature was also found to be a square relationship, suggesting that they may have survived by attaining optimal efficiency.

Next, the swimming and feeding of the colony of choanoflagellates are discussed [3]. The choanoflagellates turn their flagella inwards when exposed to light and flip their flagella outwards when it is dark. Our analysis illustrates that the inward flagellar flow is advantageous for feeding, whereas the outward flagellar flow is advantageous for swimming. Due to their morphological similarities, the pumping function of a choanocyte chamber of a sponge is also addressed [4].

Finally, we discuss nodal flow in mouse embryos, the direction of which determines the left-right axis of the body [5]. The strength of the nodal flow generated by the motile cilia acts equally on the immotile cilia located at the left and right edges of the nodal cavity. Therefore, in order to create a left-right asymmetry, the immotile cilia must sense the direction of the flow, which has been confirmed experimentally. These studies demonstrate that ciliary flow gives rise to a variety of biological functions and that fluid dynamics can provide valuable insights into biology.

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Fragmentation of plastics to form micro and nanoplastics

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Is it now well established that microplastics are pervasive in the environment and in the food chain. However, the materials physics that leads to their formation remains poorly understood. I will summarize our recent work that investigates the mechanisms by which nano- and microplastics form. Bond-breaking events in plastics result from either chemical attack (oxidation, radical attack, hydrolysis, etc) or from stress-induced mechanical degradation. In semicrystalline polymers, such as polyethylene, isotactic polypropylene and polyethylene terephthalate (that account for over 70%) of the global production of synthetic plastics, chemical attack is largely localized in the non-crystalline regions. Cleavage of tie chains that connect crystals and provide strength results in embrittlement and macroscopic failure to form micro and nanoplastics. This mode of failure to form particulate pollutants under quiescent conditions, is observed only for semicrystalline plastics but not for amorphous plastics like polystyrene. [1] I will also discuss our work on the quiescent wear processes that lead to microplastic formation in polyethylene and how this differs from the case of isotactic polypropylene. The other mode of failure is due to mechanical stresses and is observed as fabrics shed microfibers during washing, or when tyres wear out during normal use. We have demonstrated that tire wear proceed through two independent processes, resulting in two distinct populations of particulate pollutants: an aerosolized nanoplastic fraction and a larger microplastic fraction that settles under the influence of gravity. [2]

[1] N. Mendez et. al., *Nature Commun. 16, 3051 (2025).*

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Oral Presentations

(Keynote and contributed)

Active and Biological Matter (AcM+BM)

Disease-associated and functional amyloid formation through phase separation

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Abstract

Phase separation (PS) and liquid condensate formation of biological macromolecules is now becoming a proteome-wide phenomenon from bacteria to humans. PS plays a prominent role in both physiological and pathological consequences. Protein phase separation and subsequent liquid-to-solid (LS) transition have been shown to be crucial mechanisms for the nucleation of protein aggregation/amyloid formation, which are associated with various neurodegenerative disorders such as Parkinson’s and Alzheimer’s disease. Liquid condensate formation may be a generic phenomenon for proteins/polypeptides above their critical concentrations, which may be further modulated by intrinsic and/or extrinsic factors such as pH, posttranslational modifications, and other cellular conditions. However, their formation and material properties must be tightly regulated for cellular functions; alterations in these properties might be conducive to condensate malfunctions. We recently showed that alpha-synuclein phase separation into condensates, followed by their solidification, results in amyloid fibril formation. Further, LS is facilitated by several Parkinson’s disease-associated conditions, including all familial PD mutations of alpha-synuclein. In contrast, phase separation, solidification, and amyloid fibril formation by protein hormones are tightly regulated and reversible, making them ideal for storage depots. I will discuss these findings regarding functional versus disease-associated phase separation and amyloid fibril formation.

The soft matter physics of wound healing

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Abstract:

I will discuss some recent work looking quantitatively at the process of wound healing using ideas from thermodynamics, continuum and statistical mechanics. Wound healing is a highly conserved process required for survival of an animal after tissue damage. The wound repair process is not only of great interest in its own right but is also a laboratory to study complex tissue dynamics and regeneration.Many wounds involve damage to an epithelial (barrier) tissue (like skin) that separates different regions of the body of a living organism. I will describe some recent work on studying wound healing in two dimensional epithelial tissues of a fruit fly pupal wing. This epithelium was chosen because it is transparent and accessible to sophisticated imaging techniques. We use live confocal time-lapse microscopy to follow the behaviour of cells in a tissue before and after wounding. I will focus on three cell-behaviours that are generally accepted to contribute to wound re-epithelialisation: cell shape deformation, cell division, and cell migration. I will describe how we are beginning to use a combination of mathematics, physics and biology to disentangle some of the organising principles behind the complex orchestrated dynamics that lead to wound healing.

https://people.maths.bris.ac.uk/~matbl/

AcM+BM-Keynote-03

The life of a polar active polymer: progressive deformation, stretching, collapsing and knotting

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A large number of crucial biological functions in the cell are governed by polymer activity. Biological polymers become active because of the presence of molecular motors or enzymes, and synthetic polymers might come into contact with active baths or with external activation, such as magnetism or phoretic processes. In most of these cases, the activity is polar which shows to induce a progressive local deformation of the polymer chains, making a clear distinction between the conformations of head and tail segments [1]. This effect persists in melt conditions, which coexists with a local induced alignment between chain segments [2]. The number and location of the active sites on the polymer backbone play a central role in their dynamics and conformational properties [3], as well as the presence of additional interparticle interactions [4]. Globular conformations for high motor densities change to stretched ones for the more realistic moderate or low density of motors. A small difference in the position of the first motor, or the motor distribution, can also dramatically modify the polymer typical conformations in a non-monotonous intuitive manner, which can even result in partially knotted configurations.

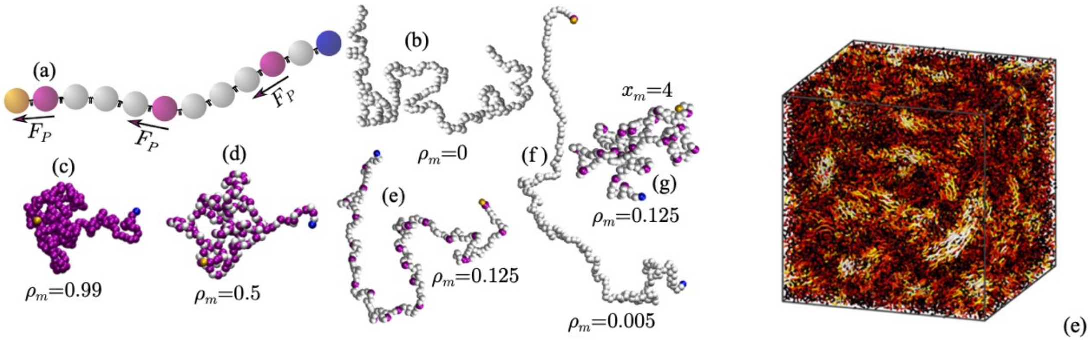

Figure 1: (a) Polar polymer sketch with head bead in yellow, purple motor beads (arrows for the force direction), blue tail, and white linker beads. Snapshot for the passive polymer is depicted for reference in (b), while snapshots from (c) to (g) illustrate globule to stretch conformations with decreasing motor densities ρ_{m}, all but (g) with x_{m}, the first motor position, at the head (adapted from Ref.[3]). (e) Simulated melt snapshot with color coded bond alignments (adapted from Ref.[2]) .

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AcM+BM-Oral-01

Control of active field theories at minimal dissipation

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Recent experimental advances allow precise control of active systems—materials that continuously dissipate energy to sustain nonequilibrium phenomena without equilibrium counterparts. Designing functional materials from such systems requires understanding how their properties can be optimally tuned by external perturbations, yet equilibrium thermodynamics offers no guidance. We develop a thermodynamically consistent optimization framework for generic active field theories. A key concept is the distinction between *protocol heat*, dissipated only during manipulation, and *total heat*, which also includes post-manipulation dissipation. We show that the total heat generically exhibits a global minimum with respect to protocol duration. Applying our framework to an active phase-separation model, we uncover scaling laws of the optimal protocol with activity and system size, and reveal how the steady-state dissipation landscape governs crossovers between distinct optimal control regimes.

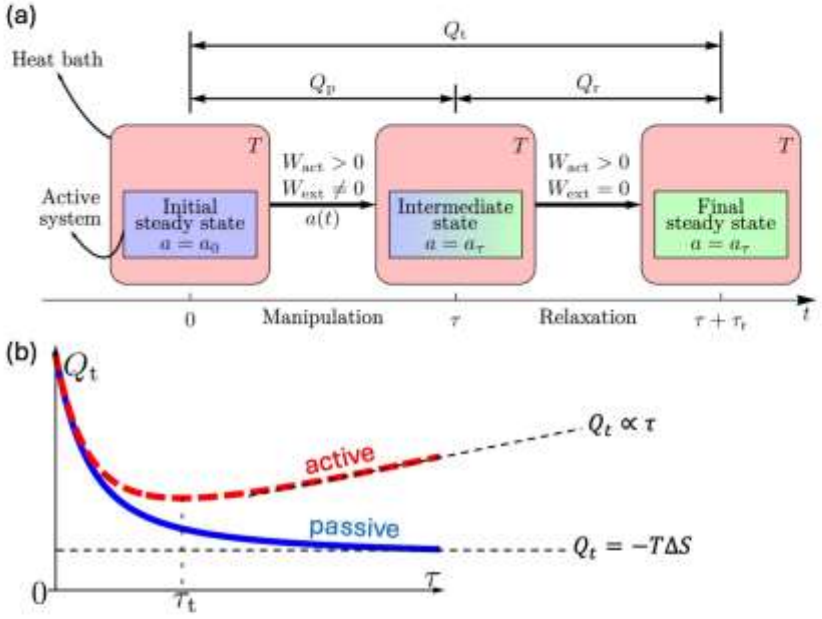

Figure 1: (a) The state of the system is changed from a_0 to a_τ over a finite duration τ. We measure the protocol heat Q_p, the relaxation heat Q_r, and the total heat $Q_t = Q_p + Q_r$. (b) The plot of the total heat Q_t as a function of protocol duration τ. For active systems, $Q_t \propto \tau$ as $\tau \to \infty$ (quasi-static limit), and for passive systems, $Q_t \to -T\Delta S$ as $\tau \to \infty$.

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Viscoelastic Response of Folded Protein Chains under Tension: Insights from Titin and Ubiquitin

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The nanomechanical response of a folded single protein—the natural nanomachine responsible for myriad biological processes—offers crucial insights into its function. The conformational flexibility of the folded state, characterized by its viscoelasticity, enables proteins to adopt different shapes to carry out their biological roles. Despite extensive efforts, direct measurements of this property have only recently become possible[1, 2]. From a nanomechanical standpoint, both internal friction and stiffness can be directly probed by deforming a single protein at a defined strain rate. To characterize a protein's viscoelasticity, it must be periodically strained while monitoring the in-phase and out-of-phase components of the resulting stress. Such measurements provide quantitative values for both the molecular stiffness and internal friction coefficient. Particularly intriguing are tandem arrays of globular proteins—such as the tiplinks formed from cadherin tetramers or the titin molecules within muscle sarcomeres—that are subject to mechanical tension under physiological conditions.

Here, we present direct and simultaneous measurements of the stiffness and internal friction of an octamer of immunoglobulin-like (Ig) domains from titin, $(I27)_8$, and of polyubiquitin chains. We find that a chain of 8 folded I27 domains exhibits measurable energy dissipation accompanied by a softening of the molecular chain. In contrast, polyubiquitin chain of 8 identical domains show neither dissipation nor corresponding softening. Interestingly, the stiffness of ubiquitin chains under high force (> 50 pN) remains constant across different lengths—behaviour inconsistent with the predictions of freely jointed chain (FJC) or worm-like chain (WLC) models of entropic elasticity. For titin, similar behaviour is observed when all octamer units occupy the mechanical intermediate state. At forces around 100 pN, the polyprotein softens considerably upon further stretching. Simulations suggest that this behaviour arises from fluctuations between the native and intermediate states of individual domains. Such viscoelastic softening may underlie titin's distinctive "force-buffer" behaviour, wherein the force required to transition domains into intermediate states is largely independent of temperature and pulling speed.

The contrasting behaviour between tandem-domain proteins with and without mechanical intermediates is noteworthy. Further investigations are needed to elucidate the physiological significance of these intermediates in proteins subjected to mechanical tension.

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The role of memory and temporal scales in activity induced interactions

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Mintu Karmakar, Wenzhou Institute of CAS
Ignacio Pagonabarraga, University of Barcelona

Equilibrium theory of colloidal mixtures relies on 'integrating out' of the degrees of freedom of one of the components resulting in renormalisation of the effective depletion interaction between the colloidal particles. Such interactions are often treated as instantaneous, however, as pointed out by van der Schoot et al. [1], depletion forces in host dispersion of differently sized colloids only decays algebraically with time, and one must be wary of treating depletion as instantaneous interaction in kinetic studies.

Active particles, from bacteria to synthetic microswimmers, must often navigate complex fluids whose viscoelastic memory fundamentally alters their motion. Here, we systematically study the effect of memory for active particle dynamics in media with long-range viscoelasticity [2]. Our exact solutions of non-Markovian Generalized Langevin Equation with a fractional memory kernels for the translation/rotation reveal distinct non-Markovian signatures with dramatic enhancement of persistence leading to a prolonged ballistic or an intermediate anomalous super-diffusive regime for linear swimmers, or prominent memory-enhanced oscillations for circling swimmers. On a more coarse-grained scale, we explore the emergence of viscoelastic-like memory effects in active depletion interactions mediated between colloidal particles embedded in active fluid comprising self-propelled active Brownian particles with aligning torque interactions. We have previously shown that Vicsek-like fluid can be globally perturbed by a single small obstacle leading to new fluid states with complex chaotic wave patterns [3]. In line with that behaviour, for two passive inclusions we observe a complex response with different dynamic regimes: from adiabatic regime with instantenous interactions (weak alignment), to a regime where the time scales overlap (strong alignment, weak propulsion), and a collective regime in which the time scale of the fluid relaxation is larger larger than the intrinsic scale of colloidal motion (strong alignment and propulsion). We observe [4] a complex dependence of the nature of the host fluid-mediated interactions on these parameters with regions of attraction and replusion at multiple characteristic length-scales and a spontaneous emergence of vorticity in the intermediate regime, where we also observe the emergence of long-range attractions analogous to the Casimir forces.

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Shaping active matter: Symmetry, confinement, and effective interactions

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Active matter systems, composed of self-driven entities that continuously consume energy to generate motion or mechanical stresses, represent a fundamental departure from the principles of equilibrium statistical mechanics. Their collective behavior arises from a complex interplay between direct interactions, hydrodynamic couplings, and the self-consistent evolution of the medium in which they are embedded. Understanding the mechanisms underlying pattern formation, self-assembly, and emergent order in these systems poses profound theoretical and conceptual challenges for nonequilibrium physics.

I will discuss the role of symmetry and confinement in the effective interactions *that* govern the organization of active systems across scales. Using minimal dynamical models, I will show that the symmetry of self-propulsion plays a decisive role in the nature of emergent structures in suspensions of self-propelled particles and in complex environments.

I will further address the role of soft confinement, such as droplets, vesicles, and phase-separating mixtures, in shaping the collective behavior of active particles. Active stresses within such environments compete with interfacial tension and other restoring forces, giving rise to enhanced interfacial fluctuations, dynamic morphologies, and, in some regimes, the stabilization of active emulsions with well-defined length scales. These phenomena illustrate how activity can arrest coarsening, control morphology, and promote the coexistence of nonequilibrium steady states.

Taken together, these results highlight how fundamental symmetry considerations and mechanical constraints can be used to rationalize and predict the emergent organization of active systems. They also point toward a unified framework for understanding the self-organization of active materials—biological or synthetic—through the balance of internal activity, confinement, and effective interactions.

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A Coarse-Grained Model for Unfolding-Driven Fibrin Mechanics

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Fibrinogen, the precursor of fibrin and a key structural component of blood clots, exhibits a highly complex architecture that gives rise to remarkable mechanical behavior. Its assembly into fibrin fibers through half-staggered packing, knob-hole interactions, and αC-region crosslinking produces a material with exceptional extensibility and nonlinear stress-strain characteristics that remain only partially understood [1,2]. To elucidate the molecular origins of this behavior, we develop an Unfolding-Incorporated Coarse-Grained Polymer model that explicitly captures domain unfolding within fibrinogen [3]. The model accurately reproduces stretching responses observed in experiments and all-atom simulations [4]. We extend this framework to fibrin fibers and networks, enabling systematic investigation of how molecular unfolding events propagate to mesoscopic and macroscopic mechanical properties. Our approach provides a predictive model for understanding the nonlinear elasticity of crosslinked fibrin gels and represents controlled, mechanistic descriptions of domain unfolding in crosslinked biopolymer networks. Beyond fibrin, the our model offers a versatile tool for studying biological and synthetic systems governed by sacrificial-bond mechanics[5].

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AcM+BM-Oral-06

Clusters, loops, lanes, and flocks: non equilibrium patterns by chemically communicating active agents.

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Nature abounds with species that communicate using chemical fields. From micron-scale bacteria to larger social insects, a wide range of organisms rely on chemical signals to convey information about resources, threats, and collective opportunities. The motion of such organisms exhibits a striking diversity of collective patterns, including static clusters, lane and highway-like structures, loops, and flocking states. Here, we develop a theoretical model inspired by Marangoni-driven self-propulsion[1], which incorporates reaction–diffusion dynamics of the chemical field and the self-propelled motion of active agents responding to local chemical signals. Using this model, we investigate the collective behavior of interacting active agents by varying key parameters such as the chemical loss rate and diffusion constant, as well as the sensitivity and motility of the agents.

Our numerical studies reveal a wide range of collective patterns observed in natural systems, which can be organized into a state space defined by the chemical loss rate and agent sensitivity, relative to the self-propulsion speed. To gain further insight, we derive mean-field equations for the density, polarity, and chemical fields and analyze the instabilities of the system. This analysis demonstrates the emergence of coupled density and polarity patterns driven by agent-generated chemical fields. Overall, our results show that a broad spectrum of collective behaviors observed across diverse organisms can be captured within a minimal theoretical framework, with potential implications for both biological systems and the design of synthetic active matter.

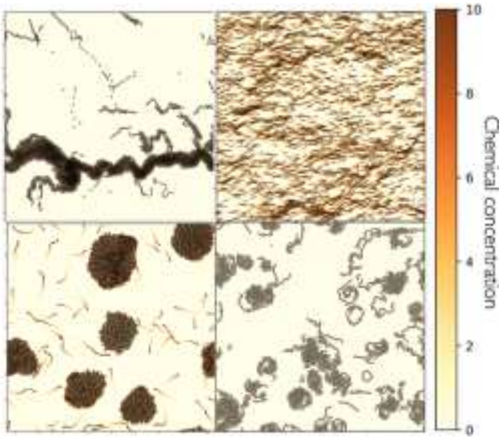

Figure 1: Lanes, flocks, clusters, and loops. Snapshots of different dynamical states shown by chemically communicating active agents

[1] P Masanta, R Sarkar, P Parmananda, R Chelakkot, *Dynamics of Marangoni-Driven Elliptical Janus Particles,* arXiv:2512.20283

Oscillating Cell Shapes: Patterns, Mechanisms, and Dynamics

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Abstract: Periodic oscillations in cell shape often mark the onset of coordinated collective behaviours, revealing how mechanical feedback and biochemical activity intertwine to drive morphogenetic pattern formation. To elucidate these processes, we develop a general coarse-grained theoretical framework: (i) a global mean-field description and (ii) an active continuum gel model that incorporates key cellular processes such as actomyosin contractility, mechanochemical feedback, and the viscoelasticity of the cell-substrate system. This approach captures diverse morphogenetic processes, from cell shape oscillations to large-scale deformations, and predicts a variety of spatiotemporal patterns, including propagating waves, oscillatory instabilities, residual strain states, and spatiotemporal chaos. Together, these formulations provide a unified theoretical framework for understanding the dynamics of the actomyosin cortex and the emergence of coordinated collective cellular motion during tissue development.

Self-propulsion and Dynamic Clustering of Photo-active Nano-sized Particles in a Brownian Environment Probed by Heterodyne Dynamic Light Scattering

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From microorganisms to synthetic particles, active systems are capable of autonomous motion and can propel themselves by harvesting energy from their environment. Scientists have designed several particle systems capable of self-propulsion with self-generated gradients and a specific response to external stimuli such as, among others, chemical sensing or light illumination. Although remarkable progress has been made in propelling micrometer-sized particles, self-propulsion of nano-sized objects following desired trajectories within a non-confined 3D Brownian environment is challenging due to low Reynolds number. Another major difficulty is technical; new experimental approaches must be implemented to track a very large ensemble of nanoparticles that are too small to be observed by optical microscopy.

Recently, we successfully demonstrated that UV-activated 65nm AgCl nanoparticles are capable to produce a directional self-propulsion by electrolyte self-diffusiophoresis. We detailed their motion using a novel light scattering method based on heterodyne detection, [1,2] a powerful interferometer allowing not only the study of Brownian motions, but also the accurate determination of absolute speeds and directions of propelled nano-objects. [1]

Another specific property of active particles is their ability to organize themselves into dynamic clusters as they move. Heterodyne DLS also unveiled the dynamics of their formation at nanoscale. Among the new perspectives on active matter offered by this approach, we will describe the first results concerning nanoparticles propelled by rotary molecular motors.

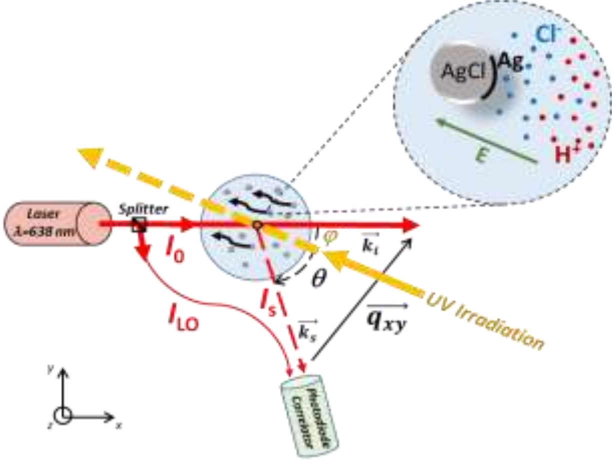

Figure 1: Principle of heterodyne dynamic light scattering and of the self-propelled motion of AgCl-NPs by UV-induced electrolyte self-diffusiophoresis. The particle scattered signal is mixed with waves from a reference local oscillator (LO). The endegenous electric field that powers the motion is due to the difference in diffusivities of the released H^+ and Cl^- ions.

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AcM+BM-Oral-09

Two particle micro-rheology of collagen gels

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Collagen type 1 is the most abundant extracellular matrix protein. Collagen exerts its role as a load bearing structure only once it is assembled into fibrils. The collection of collagen fibrils dictates the mechanical properties of the extracellular matrix in-vivo as well as of collagen gels formed in-vitro. Several collagen binding proteins such as decorin[1], are known to modify the structure of collagen fibrils. These structural alterations can affect the mechanical properties of individual fibrils[2] as well as that of the collagenous substrate, typically yielding an inhomogeneous material. Micro-rheology is a useful approach to characterize mechanical properties of such inhomogeneous soft materials[3] especially when available in limited amounts.

In this study, we investigated how decoron, the core protein of the decorin proteoglycan, affects the mechanical properties of collagen gels. Collagen gels formed in the presence or absence of recombinant decoron were macroscopically tested via parallel plate macro-rheology. Micro-mechanical properties of identically prepared gels embedded with micro-beads were investigated using a novel two-particle optical tweezer technique (**Figure 1**). In this approach, a single bead was trapped and oscillated using an optical tweezer. The displacement of the trapped (driven) beads as well as that of the satellite un-trapped (receiver) beads was monitored. These measurements were used to ascertain the local one-particle (around driven bead) and two-particle (between driven-receiver pair) shear moduli.

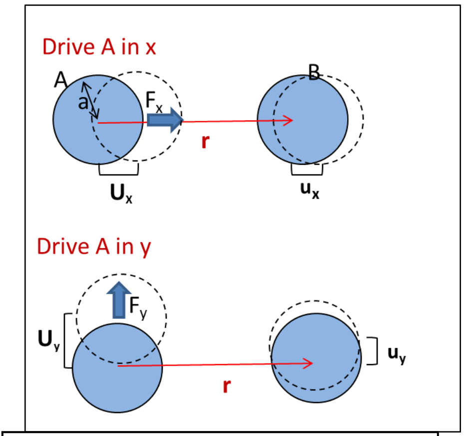

Figure 1: Two-particle micro-rheology measures displacement (U_i: U_x or U_y) of a driven bead **A** and the induced displacement (u_i) of the satellite receiver bead **B**, separated by a vector **r**.

Our results show that two-particle micro-rheology enabled coarse-grained evaluation of the mechanical environment. For large bead spacings, two-particle measurements yield moduli consistent with our measured macroscopic values. However, for small bead spacings, the derived moduli values increase as the inter-bead spacing decreases. And asymptotically, for a bead spacing of zero, our two-particle measurements reach those given by one-particle measurements, which overshoot the macroscale moduli. We elucidate how two-particle micro-rheology by optical tweezers can enable a more comprehensive characterization of mechanical properties of soft materials than achievable by conventional one-particle micro-rheology or by macro-rheology.

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Chromatin loops provide a structural basis for molecular memory

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Transcriptional activation and signalling responses often exhibit memory, persisting beyond the duration of the initiating stimulus. The physical basis of such memory, however, remains poorly understood. Here we show that chromatin looping provides a structural scaffold that enables fast transcriptional response and encodes molecular memory across signalling cycles. Using polymer-based simulations, we show that binding sites proximal to CTCF-mediated loop anchors act as stable nucleation sites for protein condensates, promoting their rapid formation. We find that looped architectures accelerate condensate formation during repeated signalling cycles and preserve condensate memory after signal decay in the form of small aggregates at persistent looped sites, suggesting a mechanism for molecular bookmarking across signalling events. Disruption of loop topology abolishes efficient nucleation and slows subsequent transcriptional activation. Together, our results identify chromatin loops as a structural basis for molecular memory, linking three-dimensional genome organisation to the persistence of transcriptional states.

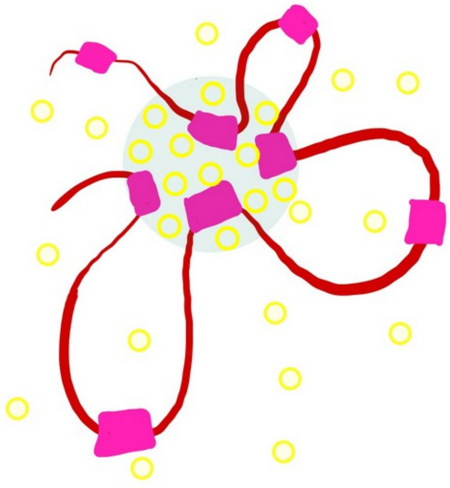

Figure 1: Chromatin structure provides a scaffold that enables fast and persistent functional response

Phase separation and viscoelastic properties of chemically active biomacromolecules

Gaurav Chauhan

Phase separation of proteins and nucleic acids can result in membraneless compartmentalization in the intracellular environment. The current theoretical and computational paradigm assumes an equilibrium concentration of biomacromolecules. This assumption may not hold up for a variety of systems with active production and degradation. Recent studies indicate that such active turnover can drive condensates into dynamic steady states, where chemical fluxes balance droplet formation and dissolution, resulting in phenomena like size selection and arrested coarsening. Here, we study the role of active degradation and production on the phase diagram of model coarse-grained polymers. By using Langevin dynamics simulations of associative polymers coupled to a kinetic Monte Carlo production and degradation scheme, we have studied the role of active production and degradation on the phase diagram. We have also studied the role of activity on droplet fusion, dynamics and interfacial tension. Activity has been shown to affect viscoelastic properties, conformations of polymers and interfacial properties. Our work helps to understand how the chemically active intracellular environment modulates biomolecular condensates.

How Cells Control Nanoscale Transport: Stability in Physiology, Disruption in Stress

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The cytoplasm of human cells behaves as a complex soft-matter system whose nanoscale physical properties directly shape biological function. Using fluorescence correlation spectroscopy, raster image correlation spectroscopy, and length-scale–dependent viscosity (LSDV) analysis, we show that the cytoplasm maintains a remarkably robust nanostructure under physiological conditions. Across diverse human cell lines and throughout the cell cycle, the effective viscosity sensed by nanometer-sized tracers follows a conserved size-dependent profile, reflecting a stable architecture composed of ~4-5 nm intercrowder gaps and ~20 nm effective crowder radii. This organization supports diffusion-driven biochemical processes by ensuring predictable transport over length scales below ~100 nm, while larger objects experience gel-like confinement imposed by the cytoplasmic mesh [1].

Under stress, however, this soft-matter system undergoes abrupt physical transformations with clear biological consequences. Starvation compresses the cytoplasmic network, reducing pore size from ~100 nm to ~30 nm and immobilizing large ribosomal subunits, effectively downregulating translation [2]. During apoptosis, nanoviscosity increases two- to four-fold within minutes, driven primarily by water efflux and volume loss, sharply slowing diffusion across all nanoscales [3]. These stress-induced transitions illustrate how cells actively or passively modulate their internal rheology to regulate metabolism, preserve genomic function, or trigger programmed cell death.

Our findings demonstrate that cytoplasmic nanostructure is not merely a passive background but a dynamic soft-matter platform linking physical transport laws with cellular physiology. Moreover, we found that routine laboratory procedures – like transfection – influence this network. Understanding these nanoscale physical transitions offers new routes to interpret metabolic adaptation, stress responses, and the physical determinants of cell fate.

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[3] A. Zgorzelska *et al.*, *Cell Rep. Phys. Sci. 6, 102927 (2025)*

Viscoelasticity of airway mucus and ciliary clearance of airway epithelia by live-cell rheometry

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Mucus plugs occlude airways to obstruct airflow in asthma. These plugs form due to mucus stiffening as a result of abnormal airway regulation or infections, which hinder the ability of cilia to clear mucus from airways. To determine how mucus rheology and mucociliary clearance ability of human airway epithelial cells (HAECs) are interrelated, we developed a magnetic disc rheometer. This instrument is able to characterize both the viscoelastic properties of mucus secreted by HAECs and the ciliary clearance ability of these HAECs under varying conditions. Its utility is demonstrated by examining the effect of two naturally occurring agents: interleukin-13 (IL-13) and prostaglandin E2 (PGE2). IL-13 is an inflammatory cytokine and is overexpressed in cases of acute asthma. It is shown to cause a transition in mucus from a viscoelastic liquid towards a viscoelastic gel, leading to diminished cilia-driven flow. PGE2, on the other hand, is a bronchodilator and anti-inflammatory agent. With PGE2 treatment normal HAECs secreted viscosified liquid mucus and had improved cilia-driven flow. Together our results show that IL-13–stimulated HAECs autonomously generate pathologic mucus and have diminished mucociliary clearance ability compared to normal HAECs, which can be restored to healthy-like behavior with PGE2.

Motility-Induced Organization of Polymers from Active Monomer Units

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Active matter is a new and rapidly growing topic that describes systems with active agents that are capable to transform the surrounding's energy into their own. There is no classical thermodynamic equilibrium and unusual effects of self-ordering and segregation can be observed. Such systems can be found on different spatial and temporal scales, ranging from bacteria and molecular motors to flocks of birds and fish swarms. But what happens if the active agents form polymer chains? Polymers are poor in entropy, and therefore more prone to self-ordering and structurization than low-molecular-weight systems. Several models of polymers with active monomer units will be used to demonstrate their peculiarities and unusual properties, including their ability to undergo co-directed collective motion [1,2], collapse under the influence of activity [3,4], and even microphase separation. In addition to possible future technological applications, we believe that these kinds of interactions may play a key role in structuring DNA in eukaryotic nuclei, including the separation into eu- and heterochromatin.

This work was financially supported by the RSCF (project 23-73-00089).

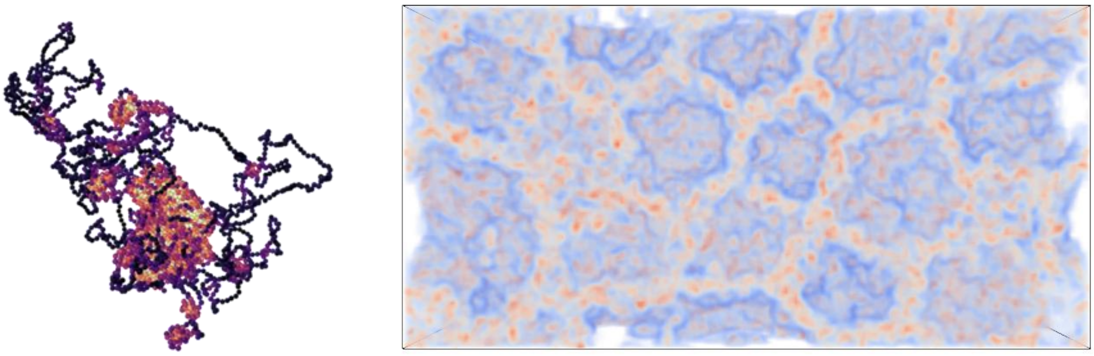

Figure 1. Example of polymer system with active monomer units as a single chain (left) and unusual microphase separation in a concentrated solution (right).

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AcM+BM-Oral-15

Mechanical Regulation of Cancer Invasion by the Cell Surface Glycocalyx

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Cancer progression and metastasis are governed by coupled mechanical and biochemical interactions within the tumor microenvironment, with the glycocalyx emerging as a critical but underexplored regulator. Though the bulkiness of the glycocalyx has been implicated in enhancing invasiveness and drug resistance, the physical mechanisms by which the glycocalyx mediates these effects remains incompletely understood. By approximating the glycocalyx as a poroelastic material, using FEM simulations of indentation of a cell by a spherical probe, we show that the glycocalyx regulates stress propagation through the cell by absorbing a large fraction of applied loads, resulting in pronounced stress relaxation and shielding buildup of stresses on the nucleus. We further demonstrate that variations in glycocalyx thickness and stiffness strongly regulate poroelastic dissipation and stress transmission across different mechanical environments. Figure illustrate Cells without a glycocalyx (solid blue curve) exhibit higher peak forces and slower relaxation, indicative of direct load transfer to the cytoplasm. In contrast, inclusion of the glycocalyx (red dashed curve) markedly reduces peak force and accelerates relaxation, consistent with efficient poroelastic dissipation within the glycocalyx layer. Moreover, during Confinement migration, the glycocalyx absorbs a substantial portion of applied mechanical loads, thereby buffering stress transmission to the cytosol and nucleus. Under cyclic confinement, force peaks and loading duration increase, while the presence of the glycocalyx alters the temporal evolution and spatial distribution of transmitted stresses. These results establish the glycocalyx as a poroelastic, energy-dissipating layer that governs the early mechanical response and provides mechanical protection under invasion-relevant loading conditions. Together, these findings offer mechanistic insight into how the glycocalyx mitigates invasion-associated mechanical stresses, promotes nuclear integrity, and enhances cancer cell survival during metastatic transit.

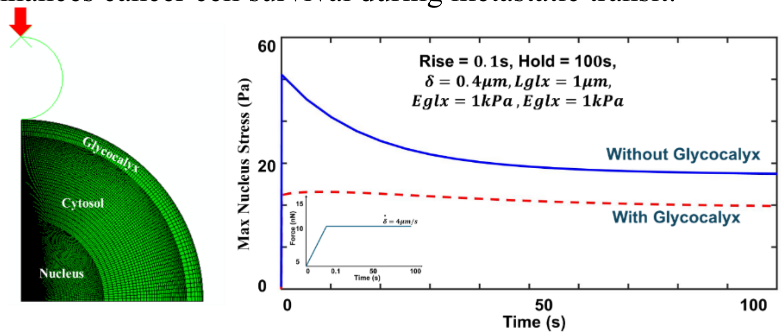

Figure 1: Glycocalyx Regulates Stress Transmission to the Nucleus
(a) Finite-element model of AFM-style indentation of a cancer cell, (b) Simulated force–time (stress-relaxation) response for a 0.1s loading ramp followed by a 100s hold.

3D bulk gels and microfluidics: *in vitro* pancreatic tumor models for studying T cell migration.

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Immunotherapy has emerged as a promising approach for treating cancer, however its efficacy against pancreatic tumors has been limited[1] due to its dense stroma. Because of this, many regions of pancreatic tumor, have areas within the tumor that exclude anti-tumor immune cells[2]. To be effective, cell based immunotherapies are required to be in close proximity with the cancer cells[3]. Therefore, we need to define mechanisms used by therapeutic T cells to navigate effectively in some tumor regions and barriers that limit their infiltration in other regions of tumor microenvironment (TME). In this work, we have advanced our knowledge of T cell migration through the design of complex TMEs such as bulk collagen gels and microfluidic devices and by analyzing T cell dynamics in these 3D engineered *in vitro* platforms, that can replicate key TME features of pancreatic ductal adenocarcinoma (PDA). Using imaging techniques such as multiphoton excitation (MPE) and second harmonic generation (SHG), we have monitored migration of engineered mesothelin reactive chimeric antigen receptor (CAR) T cells through these environments and their interactions with pancreatic tumor spheroids. Quantitative analysis of interactions between CAR-T cells and carcinoma cells, in terms of velocity, directionality and persistence were performed, with the aim of utilizing these phenotypes as "design criteria" for development of more effective T cell therapies. Therapeutic efficacy of these T cells was also evaluated in 2D killing assays and then 3D assays of increased complexity, both of which revealed mesothelin specific cancer cell death. Overall, we have tried to define physical/molecular mechanisms that result in immunotherapy resistance against pancreatic cancer, and we anticipate that this work will be applicable to other solid tumors with similar challenges and address key unanswered question in cancer biochemistry.

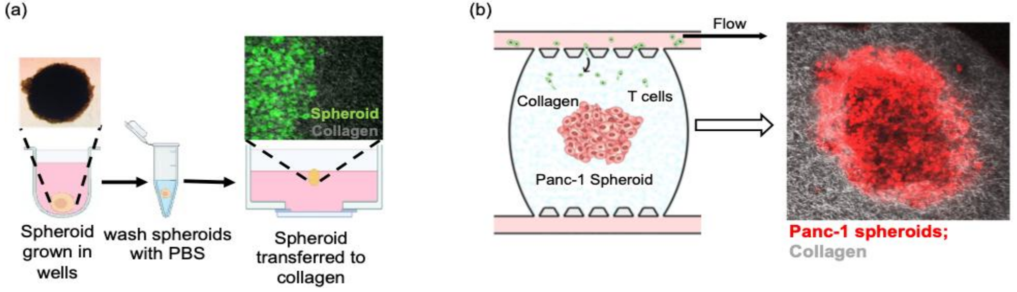

Figure 1. In vitro models for pancreatic cancer (a) Bulk gels (b) Microfluidic devices.

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AcM+BM-Oral-17

Understanding the nonlinear behaviour of living tissue: mechanistic models & dynamics

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We present some of our work on modelling living systems through mechanical analogies. We focus on two distinct aspects – dynamics of fluid transport in xylem, and understanding the nonlinear behaviour of muscle tissue. Using a modified Bosanquet equation, we account for the effect of charged species in the sap, friction due to helical structures on the xylem wall, etc,, and show how oscillations are induced in the system depending upon the relative magnitudes of capillary to hydrostatic forces & friction in the system. Scaling power-laws for the stabilization time for the sap column are obtained. Including transpiration, changes system stability to that around a nonlinear center & explains several other features seen in actual sap transport [1].

In an attempt to understand muscle contraction and behaviour in physiological conditions, we follow two distinct approaches in parallel that we then bring together. First, we study the behaviour of a confined, semiflexible (wormlike) polyelectrolyte chain, using a double-screening mean-field theoretical [2] approach, where screened electrostatic and excluded volume interactions are included, with restrictions on chain conformations being imposed by adopting the Odijk deflection length [3]. The dependence of the renormalized Kuhn length and chain stiffness are calculated as functions of various parameters, across varying salt and monomer concentrations and molecular weight. We map this to our theoretical studies [4-6] of mechanical, nonlinear oscillators with nonlinear stiffness, in an attempt to understand and predict the complex dynamical response of living tissue. While the macromolecular approach enables us to describe system behaviour under biological relevant physiological parameters such as salt concentration, the dynamical systems theoretical approach gives us a handle on the changing dynamical regimes that the system will display for varying displacements, enabling us to tune the system to desired dynamical regimes by appropriately adjusting salt concentrations.

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DNA based programmable nanodevices to instruct biological systems

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Abstract : My laboratory ask how nanometer-sized biomolecules transmit and integrate information across much larger length scales of the orders of cells and tissues. We seek to explore how collections of macromolecules work together to establish a common functional system like cellular pathways, organelles, living cells and further into tissues, organs and entire organisms. Different biomolecules establish long-range orders in living systems by self-assembling into much larger structures, such as molecular complexes, membranes, and cytoskeletal organelles, intra- and inter-cellular contacts, and long range contacts. The main theme of our lab will be understand the assembly principles of biological systems and the roles they play in living cells, tissues and full organisms...and further developing technologies to modulate the same.

To address these problems, we adapt multidisciplinary, bottom-up approach using DNA nanotechnology. DNA has immense potential to arrange the matter at nanoscale with extreme robustness and spatial specificity. The compatibility of DNA to interface with other biomolecules like proteins, carbohydrates, lipids, small molecules make DNA a natural choice of material for bottom-up self-assembly. Thus, we will merge the complex programmability of DNA nanotechnology with the structural and functional diversity of other biomolecules. Our interdisciplinary research, along with national and international collaborations with experts, will leverage expertise from chemistry, nanotechnology, biophysics, biology, engineering, and medicine.

The overarching goal of the my team would be to translate laboratory findings into the development of new therapeutic strategies.

Keywords: Structural DNA nanotechnology, 3D cages, Monofunctionalized quantum dots, Single particle tracking, Super resolution live cell microscopy, Biomedical and translational applications.

Role of the motor density and distribution on polar active polymers

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Polar polymer activity underlies numerous cellular processes driven by molecular motors or enzymes. Active polymers with activity on all constituent monomers display compact globular structure, while polymers with only head activity are known to result in stretched configurations. However, most biological and synthetic polymers feature activity localized in just a few sites, a scenario that significantly differs from both previous limits. We investigate how the density and distribution of motors critically influence the conformational and dynamical properties of polar active polymers. Using overdamped Langevin dynamics simulations, we show globular conformations for high motor densities change to stretched ones for the more realistic moderate or low density of motors. Interestingly, the polymer's velocity exhibits a non-monotonic dependence on motor density, with maximum propulsion at intermediate densities. Furthermore, the location of the first motor profoundly impacts polymer conformations; even a slight shift leads to drastic differences between coiled and stretched states. Our findings reveal that motor placement and density govern the structural transitions, characteristic timescales, and propulsion dynamics of polar active polymers, which will have numerous practical implications in the design and understanding of active synthetic and bio-polymers.

S. Jaiswal et. al, "*Critical role of the motor density and distribution on polar active polymers*" Physical Review Research (2026)

Unravelling cellular mechanosensing on cell-scale stiffness gradients

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Many key biological processes including neurogenesis, angiogenesis, and cancer metastasis are modulated by the mechanical properties of the extracellular matrix (ECM). ECM stiffness spans several orders of magnitude across tissues, and cells actively sense and transduce these mechanical cues through integrin-mediated adhesions and the actomyosin cytoskeleton. Spatial variations in matrix rigidity can elicit directed cell migration (durotaxis) and modulate force generation, polarization, and signalling. Despite significant progress in fabricating stiffness-gradient substrates, generating high magnitude stiffness gradients at the level of cellular length remains a major technical challenge. In this talk, I will present a fabrication strategy developed in our laboratory that leverages controlled topographical modulation to engineer substrates with steep and spatially well defined stiffness gradients. Local elastic moduli are quantitatively mapped using atomic force microscopy, enabling resolution of gradient profiles with subcellular precision. Finally, I will discuss how cells sense and respond to these steep mechanical landscapes, focusing on cytoskeletal polarization dynamics, and gradient sensitivity, providing mechanistic insights into cellular mechanosensing under physiologically relevant mechanical heterogeneity.

AcM+BM-Oral-21

Differential contributions of microtubules and spectrins to axonal mechanics

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Axons grow to extreme lengths and hence are subjected to large stretch deformations during limb or other bodily movements. Axons in the brain too undergo significant deformations even during normal activities, and can be damaged causing concussion or traumatic brain injury during head impacts. Have axons evolved special strategies to withstand large deformations? To this end, we investigate the mechanical responses of microtubules and the actin-spectrin periodic scaffold in axons. Our experiments suggest that microtubules are able to relax mechanical stress by unbinding of crosslinks, whereas the spectrin scaffold can buffer excess tension by unfolding of spectrin repeats--triply folded alpha helices connected by linker domains. This, in effect, makes the parallel array of microtubules behave elastically at short times (sudden deformations) and fluid-like at long times. The spectrin scaffold, on the other hand, behaves as a non-linear viscoelastic solid. We'll discuss the functional consequences of these differential contributions and how it might help us better understand axonal susceptibility to injuries like concussion, traumatic brain injury and stretch injuries to nerve fibers.

Wetting-mediated extracellular phase separation drives cell adhesion

Jiaxing Yuan

Cells must efficiently locate and engage for tissue formation and immune coordination, yet classical receptor-ligand binding is limited to nanometer distances and is inherently slow. Here, we uncover a previously unrecognized physical principle: Liquid-like Adhesion by Phase Separation (LAPS). This process creates dynamic wetting layers on cell surfaces, functioning as “liquid bridges” that enable robust, long-range cell capture across tens of micrometers. Remarkably, this wetting-mediated attraction remains effective at nanomolar concentrations—conditions where bulk phase separation would not be expected—and facilitates high-fidelity cell sorting through competitive wetting. By integrating aqueous two-phase systems, endogenous proteins (Galectin-3, CCL5), and fluid-particle-dynamics simulations, we demonstrate that extracellular liquid-liquid phase separation not only mediates long-range cell capture but also acts as a physical catalyst for contact-dependent signaling. These findings establish extracellular phase separation as a key physical principle complementing molecular recognition in multicellular systems, offering new opportunities for understanding immune response, tissue morphogenesis, and therapeutic strategies targeting the extracellular environment.

The physical consequence of sperm gigantism

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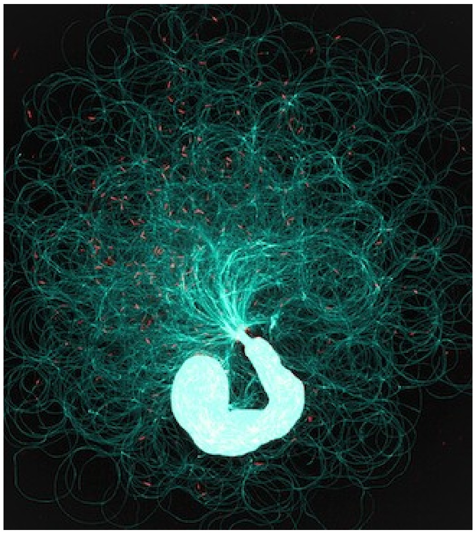
The male fruit fly produces ∼ 1.8 mm long sperm, thousands of which can be stored until mating in a ∼ 200 μm sac, the seminal vesicle. While the evolutionary pressures driving such extreme sperm (flagellar) lengths have long been investigated, the physical consequences of their gigantism are unstudied. Through high-resolution three-dimensional reconstructions of in vivo sperm morphologies and rapid live imaging, we discovered that stored sperm are organized into a dense and highly aligned state. The packed flagella exhibit system-wide collective 'material' flows, with persistent and slow-moving topological defects; individual sperm, despite their extraordinary lengths, propagate rapidly through the flagellar material, moving in either direction along material director lines. To understand how these collective behaviors arise from the constituents' nonequilibrium dynamics, we conceptualize the motion of individual sperm as topologically confined to a reptation-like tube formed by its neighbors. Therein, sperm propagate through observed amplitude-constrained and internally driven flagellar bending waves, pushing off counter-propagating neighbors. From this conception, we derive a continuum theory that produces an extensile material stress that can sustain an aligned flagellar material. Experimental perturbations and simulations of active elastic filaments verify our theoretical predictions. Our findings suggest that active stresses in the flagellar material maintain the sperm in an unentangled, hence functional state, in both sexes, and establish giant sperm in their native habitat as a novel and physiologically relevant active matter system [1].



Confocal image showing *D. melanogaster* sperm - heads in red, tails in cyan - spewing out of the seminal vesicle (SV), highlighting the sperm's enormous length and their dense packing in the storage organ

Reconstituting active and dynamic steady-states of actin-based cellular architectures

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Cytoskeletal architectures in cells, and particularly actin-based ones (lamellipodia, stress fibers, cytokinetic rings, etc.) undergo continuous self-renewal, with their individual components constantly dissociating, recycling and reassembling, while at the same time contributing to an overall stable structure. This allows different subcellular networks of the cell to be dynamically regulated, providing them with the flexibility to grow, shrink, appear and disappear as needed. Hence, actin architectures are in a "dynamic steady state" (DSS), characterized by the continuous nucleation and growth of filaments, balanced by their disassembly and recycling. Active contraction by myosin motors further contributes to maintaining stable yet active and dynamic architectures. Due to the interdependencies of all these mechanisms, investigating their properties in cells is challenging. In vitro reconstituted networks, based on the use of a minimal set of purified proteins, offer a powerful alternative allowing precise, modular control over individual components to reveal principles underlying DSS formation and maintenance. A purely recycling-based actin DSS has been recently achieved [1]. However, in the presence of myosin, reconstituted actomyosin networks typically undergo only brief, transient contractions.

Here [2], we present the reconstitution of contraction-based actin networks that instead self-organize into a dynamic steady state, ceaselessly flowing microscopically and yet maintaining a stable and steady macroscopic architecture. Using lipid-coated microdevices to confine and guide network assembly and taking advantage of both myosin-based force generation and cofilin-based recycling of actin monomers, we assemble minimal yet realistic actin architectures in DSS, both in the presence and in the absence of actin turnover. Reconstituted architectures, all based on a balance between actin transport, contraction and recycling, include networks that contract continuously, or exhibit pulsed and even spiral-like contraction waves, as observed in cells. Using the flexibility of bottom-up reconstitution, we identify conditions leading to such active steady states, dissect the microscopic dynamics giving rise to them and test their robustness. These results pave the way to a more mechanistic understanding of cellular actin architectures.

[1] A. Colin et al, *The EMBO Journal 42, EMBJ2022112717 (2023)*

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Emergent collective behavior of chiral active particles with polar alignment and visual perception

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Most self-propelled particles follow curved or fluctuating paths due to environmental interactions, shape asymmetry, or intrinsic torques. Here, we explore the collective dynamics of chiral intelligent active Brownian particles (iABPs) [1] that combine polar alignment with vision-based sensing. By varying the ratio of alignment to visual maneuverability, the vision angle, and the reduced chirality (ω/D_r), we construct a phase diagram exhibiting diverse collective states - spinners, vortices, ripples, worm-like swarms, rotary clusters, and irregular aggregates. Chirality critically governs their morphology: high chirality yields dilute or compact spinning clusters, while moderate to low chirality produces cohesive yet dynamic patterns. Ripple loops emerge as a distinct state, characterized by expanding ring-like motion driven by outward torques and sustained only when both particle number and visual maneuverability are large (as shown in Figure1). Structural and dynamical measures, including polarization, pair correlations, mean-square displacement, and orientation correlations, reveal clear signatures distinguishing these phases. Overall, our results show how chirality, non-reciprocal perception, and alignment together generate collective states inaccessible to non-chiral systems, with implications for chiral active matter [2] in biological and synthetic matter.

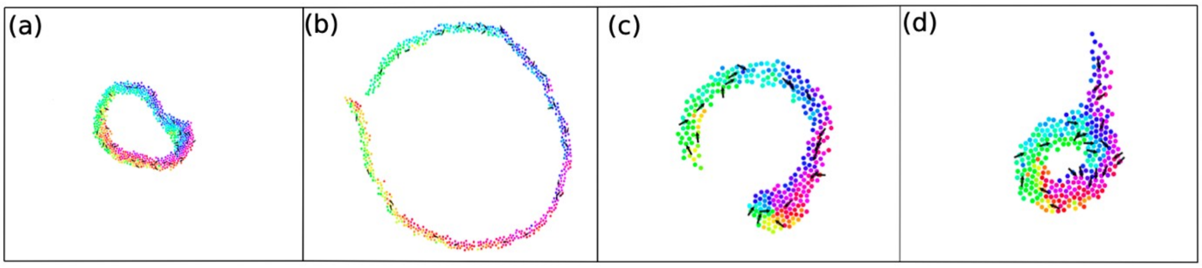

Figure1: Sequence of snapshots showing ripple dynamics: loop formation, expansion and breakup, followed by the emergence of a new loop.

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Activity-driven dynamic smectic order formation in deformable cell monolayers

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Cell monolayers exhibit both short- and long-range orientational order, which can be spontaneously created or disrupted through continuous cell rearrangements. These rearrangements originate from local mechanical stresses and can also actively generate mechanical stresses. Such active stresses are believed to play a crucial role in tissue reorganization and developmental processes. Despite this, it remains unclear how cells spontaneously modify their collective order and generate dynamic patterns in densely packed environments. In this work, we introduce an active deformable cell model that represents cells with arbitrary shapes, going beyond conventional polygon-based Voronoi or vertex models. Each cell is modelled as a ring of beads with conserved area and perimeter. Cell–cell interactions are mediated by apolar active forces that depend exclusively on the deformation of neighbouring cells and are regulated by an activity parameter. These forces act along the local contact normal and vanish in the absence of cell–cell contact. The activity parameter controls both the magnitude and direction of the contact-induced forces while ensuring that the net active force in the system remains zero. In addition, the strength of cell–cell adhesion can be independently tuned. We study the collective dynamics of cell monolayers by systematically varying the activity level and the degree of confluency. Our simulations reveal the emergence of local, dynamically evolving smectic-like order and an activity-driven unjamming transition. Furthermore, we observe a non-monotonic dependence of local orientational order on activity. We characterize the evolving tissue organization by analyzing correlation times and spatial correlation lengths. Together, these results underscore the fundamental role of activity-dependent collective dynamics in maintaining tissue integrity and shaping multicellular organization.

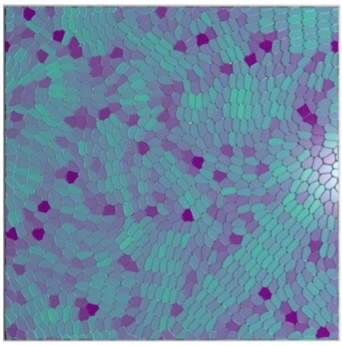

Figure 1: A snapshot of the simulation of cell-monolayer that exhibits local smectic order.

Spontaneous Hole Formation in Cell Monolayers Emerges from Collective Cell Motion

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Epithelial tissues form protective barriers lining organs, vessels, and cavities, making their integrity essential for proper function. However, mechanical stresses can compromise tissue structure, sometimes leading to fracture. While typically detrimental, fractures may serve functional roles in some organisms. For example, Trichoplax adhaerens generate fractures in the epithelium through their own motility, potentially facilitating asexual division. This process arises due to collective cell flows that localize stresses and strains, leading to tissue rupture.

Similar stress localization and fracture behaviour has been observed in vitro for tissues of MDCK cells, where fracture and rich hole dynamics occur as substrate stiffness decreases. To explore these phenomena, we present a continuum multi-phase field model that incorporates internal dissipation. Each cell is represented by a continuum density field, governed by free-energy minimization and overdamped force balance. Internal dissipation is captured by a viscosity-like term linked to the relative velocities of neighbouring cells, while a nematic director models an active dipolar forcing that promotes cell shape anisotropy.

Our results show that decreasing substrate friction enhances cell-cell velocity correlations, leading to active turbulence. In this regime, topological defects in the nematic director field form and annihilate dynamically, sometimes generating localized high-stress regions and spontaneous hole formation. We explore how the fate of these holes—whether they close or persist—depends on the tissue's elasticity and cell activity. Our findings highlight the interplay between epithelial tissues' elastic and viscous properties, shining light on the role of collective flows in regulating tissue integrity.

Active-bath mediated forces between colloidal particles: direct force measurements and dynamical signatures

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Interactions between passive colloids immersed in active suspensions can resemble equilibrium depletion attraction in appearance, but originate from fundamentally different, nonequilibrium mechanisms such as swimmer–particle collisions, hydrodynamic flows and active stresses [1]. Previous experimental and numerical studies reported short-range attractions, more recent work emphasized a strong dependence of the effective interaction on constraints [2].

We report direct measurements of the interparticle force between colloids immersed in a suspension of motile Escherichia coli, and combine these force data with structural and dynamical probes: the pair correlation function g(r), single-particle (self) diffusion, and collective diffusion coefficients. Force measurements were performed using a calibrated micromechanical approach (optical-tweezer), while particle tracking provids the diffusion and g(r) data. These measurements reveal a many-body contribution to the effective interactions and link it to emergent collective behavior.

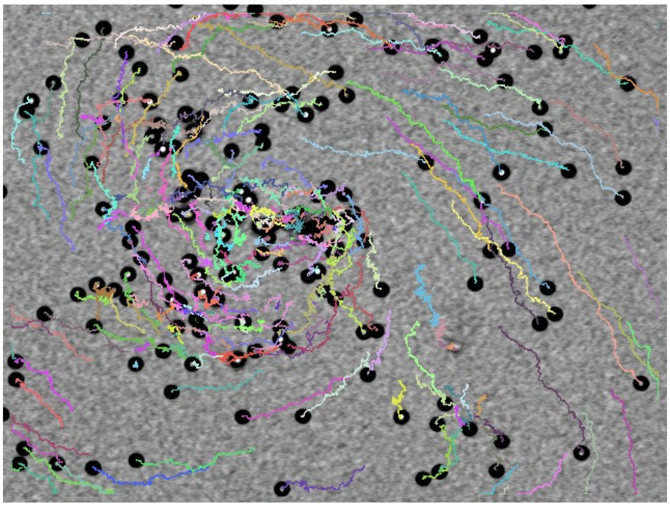

Figure 1: Large-scale flow patterns of colloidal particles. Lines indicate particle trajectories. The image width is 200 μm.

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AcM+BM-Oral-29

Glassy dynamics in epithelial tissues emerges through crowding and mechanochemical feedback

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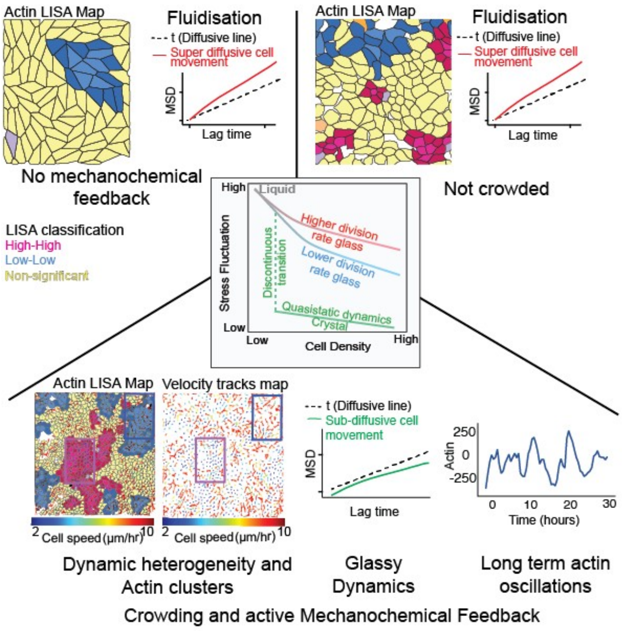
Glassy dynamics in active biological cells remain a subject of debate, as cellular activity rarely slows enough for true glassy features to emerge. In this study, we address this paradox of glassy dynamics in epithelial cells by integrating experimental observations with an active vertex model. We demonstrate that while crowding is essential, it is not sufficient for glassy dynamics to emerge. A mechanochemical feedback loop (MCFL), mediated by cell shape changes through the contractile actomyosin network, is also required to drive glass transition in dense epithelial tissues, as revealed via a crosstalk between actin-based cell clustering and dynamic heterogeneity in the experiments. Incorporating the MCFL into the vertex model reveals that glassy dynamics can emerge even at high cellular activity if the strength of the MCFL remains high. We show that the MCFL can counteract cell division-induced fluidisation and enable glassy dynamics to emerge through active cell-to-cell communication. Furthermore, our analysis reveals the existence of novel collective mechanochemical oscillations that arise from the crosstalk of two MCFLs. Together, we demonstrate that an interplay between crowding and active mechanochemical feedback enables the emergence of glass-like traits and collective biochemical oscillations in epithelial tissues with active cell-cell contacts.



Hydrodynamic Signatures in Non-monotonic Lagrangian Dynamics of Bacterial Suspensions

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Bacterial suspensions are a paradigmatic example of active matter, exhibiting persistent motion at low densities, collective turbulent-like dynamics at intermediate densities, and arrested (glassy) behavior at high densities. Despite this richness, the microscopic mechanisms governing the crossover between these regions – especially the interplay between the hydrodynamic interactions and the contact interactions – remain poorly understood. Here, we probe these transitions by tracking the dynamics of Lagrangian tracers in thin bacterial suspensions of different concentrations spanning isolated, collective and arrested regimes (Fig.1a). By analyzing the overlap functions constructed from mean square displacements for probes of varying size a, we uncover a qualitative change in tracer relaxation (Fig. 1b). At low concentrations, relaxation is purely exponential (stretching exponent $\beta \approx 1$) consistent with the uncorrelated motion. In the collective regime, relaxations become compressed ($\beta > 1$), reflecting strongly correlated dynamics characteristic of active turbulence. At high concentrations, relaxation becomes stretched ($\beta < 1$) signaling heterogeneous arrested dynamics. Remarkably, the relaxation time exhibits a non-monotonic dependence on the length scale following $\tau \sim a^{\delta}$ (Fig. 1c). At low densities, $\delta \approx 2$ consistent with diffusive motion. With increasing concentration, δ decreases and saturates at $\delta \approx 1$ in the collective regime, a scaling indicative of long-range hydrodynamic interactions. Upon further densification, δ increase again as dynamics become sub-diffusive. These observations reveal hydrodynamic interactions as a key control parameter mediating the crossover between isolated, collective and arrested states in active bacterial suspensions.

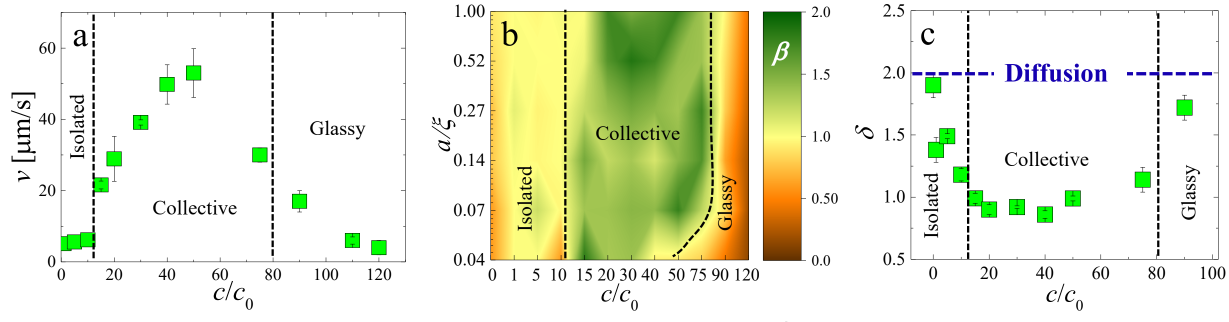

Fig 1: (a) Mean velocity as a function of bacterial concentration (c/c_0) shows three regimes separated by vertical dashed lines, where $c_0 \approx 10^8$ cells/mL. (b) The exponent β as a function of bacterial concentration (c/c_0) and probe scale a, (normalized with the flow correlation length ξ). (c) The scaling exponent δ as a function of c/c_0. The horizontal blue dashed line at $\delta = 2$ corresponds to diffusive processes.

Dynamics of an Algae-Bacteria Inhomogeneous Active Suspension

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Microorganisms inhabit highly fluctuating environments and survive in low-nutrient resource bath. It is recognized that symbiotic relationships between microbes play a vital role in their survival. The existence of such interaction raises general questions about the spatio-temporal dynamics of nutrient exchanges. Here we experimentally and theoretically examine a model system of this problem: *bacteria*, an obligate microbe capable of chemotactic response towards the green *algae*. Even in this simplest arrangement in a localized domain, we find a complex dynamics involving nutrient exchanges, enhanced algal diffusivity due to the bacteria, and a stochastic version of "flux expulsion".

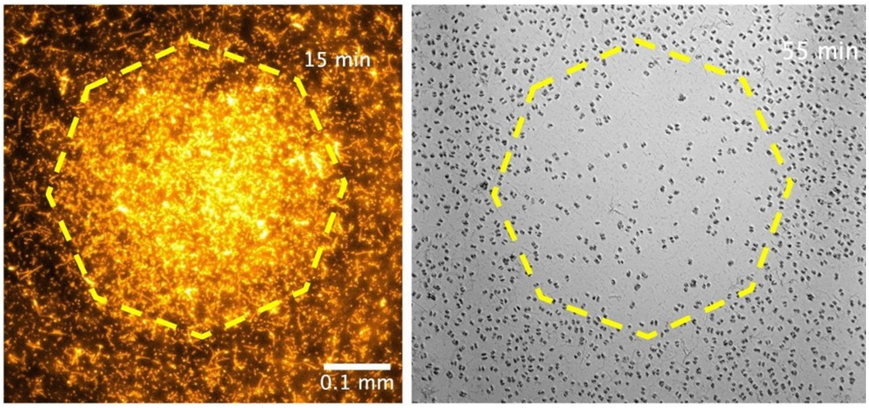

Figure 1. A shaft of light indicated by yellow octagonal ring illuminates a thin suspension of non-motile algae and motile bacteria. (a) Algae photosynthetically produces oxygen when illuminated driving the chemotactic influx of fluorescently labelled bacteria. (b) Flux expulsion of the algae from the same area.

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Metabolically driven flows enable exponential growth in macroscopic multicellular yeast

Nishant Narayanasamy
National Center for Biological Sciences

The ecological and evolutionary success of multicellular lineages stems substantially from their increased size relative to unicellular ancestors. However, large size poses biophysical challenges, especially regarding nutrient transport: These constraints are typically overcome through multicellular innovations. Here, we show that an emergent biophysical mechanism—spontaneous fluid flows arising from metabolically generated density gradients—can alleviate constraints on nutrient transport, enabling exponential growth in nascent multicellular clusters of yeast lacking any multicellular adaptations for nutrient transport or fluid flow. Beyond a threshold size, the metabolic activity of experimentally evolved snowflake yeast clusters drives large-scale fluid flows that transport nutrients throughout the cluster at speeds comparable to those generated by ciliary actuation in extant multicellular organisms. These flows support exponential growth at macroscopic sizes that theory predicts should be diffusion limited. This demonstrates how simple physical mechanisms can act as a “biophysical scaffold” to support the evolution of multicellularity by opening up phenotypic possibilities before genetically encoded innovations.

AcM+BM-Oral-33

How to propel efficiently in viscoelastic media

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Microswimmers often exploit chirality to convert rotational motion into translational movement, displaying distinct behaviors in complex fluids compared to Newtonian fluids. However, the mechanisms governing these differences remain unclear. In this study, we clarify the underlying physics driving the unique behaviors of microswimmers in Newtonian and non-Newtonian fluids using the SP method [1]. We reveal that the enhanced speed of chiral swimmers arises from the Weissenberg effect, which is induced by normal stress differences generated by chiral flows. Furthermore, we identify swimmer-specific normal stress differences in viscoelastic fluids and show that swimming speed varies depending on whether the swimmer functions as a pusher or a puller. Additionally, we explore the hydrodynamic interactions between pairs of chiral squirmers. When aligned parallel (Fig. 1(a), (c)) or perpendicular (Fig. 1(b), (d)) to their swimming axis, they exhibit tendencies to either separate or approach [3]. **Using these findings, we aimed to design a propeller capable of efficient propulsion through viscoelastic fluids.**

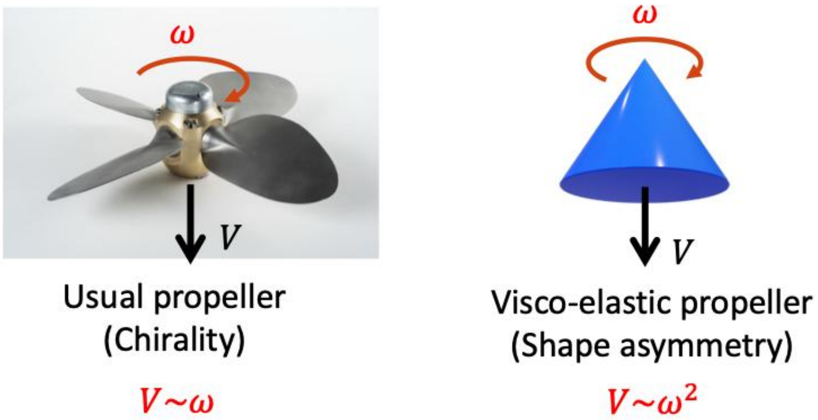

Fig.1 Schematic illustrations for an usual propeller (left) and and a viscoelastic propeller (right).

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[4] T. Kobayashi and R. Yamamoto, J. Fluid Mech., 1013, A42 (2025).

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Active Mucus-Cilia Hydrodynamic Coupling and Interfacial Rheology Govern Airway Clearance

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The airways are protected by mucus, a complex fluid transported along the epithelial surface by the coordinated beating of millions of microscopic cilia, hence the name of mucociliary clearance. Its impairment is associated with all severe chronic respiratory diseases. Yet, the relationship between ciliary density, mucus rheology, and the spatial scale of mucus transport is still unclear. Furthermore, the mechanisms that drive ciliary-beat orientations and coordination are much debated. We combine experimental physics, on in-vitro reconstituted human bronchial epithelia, with computational fluid dynamics. This enable us to identify two critical physical mechanisms necessary for an efficient clearance.

First, investigating the collective organization of cilia, we show that mucus swirls and circular orientational order of the underlying ciliary beats emerge and grow during ciliogenesis, until a macroscopic mucus transport is achieved for physiological ciliary densities. Crucially, we demonstrate that cilia–mucus hydrodynamic interactions are the governing mechanism for this collective behavior, as the macroscopic beat order is lost and recovered upon removing and adding mucus, respectively. We propose a hydrodynamic model that successfully predicts a phase diagram of mucus transport in accordance with the experiments.

Second, we address the role of mucus rheology on transport velocity. We show that cilia propel mucus efficiently across a broad range of bulk properties, from a viscoelastic fluid to an elastic solid. This striking result reveals that bulk mucus rheology is not the primary determinant of clearance failure. Instead, we demonstrate that the efficiency of mucociliary clearance is critically governed by the hydration state of a lubrication layer at the cilia-mucus interface. A hydrodynamic model, informed by measured ciliary beat patterns, allows us to infer the specific properties of this crucial interfacial layer under both actively transporting and arrested mucus conditions.

Together, these findings offer a fundamental physical understanding of bronchial clearance and provides a robust, quantitative platform to test drugs and mucolytic agents and to develop predictive *in-silico* models.

Motility-Gated Chemical Deposition Drives Re-entrant Collapse and Network Formation in Active Walkers

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Complex spatial organisation in biology, ranging from trail formation to tissue-like networks, can arise from purely local interactions coupled to chemical signalling. We study a minimal mechanism based on motility-gated chemical deposition and delayed chemotactic feedback: agents deposit a chemical only while moving, and their subsequent motion is biased by local chemical gradients while the chemical evaporates/decays.

For a single active walker on a lattice, finite-time structural measures (radius of gyration) reveal a non-monotonic change in trajectory extension with deposition rate, consistent with a coil-globule-like collapse, and re-entrant behaviour in the deposition–evaporation parameter space. The dynamics show anomalous mean-squared displacement at intermediate times, returning to normal diffusion asymptotically. A mean-field theory captures the resulting effective diffusivity.

Extending to many agents, the same feedback generates a rich phase diagram with uniform states, sparse/dense system-spanning networks, and phase separation, including re-entry into uniformity at low decay. A coupled continuum model reproduces these transitions via linear stability criteria.

AcM+BM-Oral-36

Multi-Functional Microparticles by Templating Phase Nuclei in Evaporative Liquid-Liquid Phase Separation

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Targeted delivery using active microcarriers is a promising strategy in biomedicine and environmental remediation. Effective targeting requires each individual carrier particle to integrate multiple functional entities along with payloads that enable navigation in complex environments.

Here, we introduce a facile method for producing biocompatible microparticles, comprising polymers, proteins, or protein-polymer hybrids, that encapsulate multiple functional components. The method relies on evaporation-induced liquid–liquid phase separation (LLPS) within aqueous two-phase systems (ATPS). We use two systems: polyethylene glycol (PEG)/dextran (DEX)/chitosan (CS) and bovine serum albumin (BSA)/PEG mixtures. By chemically tuning the dynamics during evaporation, we generate nucleated microdroplets that spontaneously encapsulate enzymes, nucleic acids, magnetic nanoparticles, or a combination of these, and subsequently solidify into stable particles. As a proof of concept, we demonstrate the active dynamics (super diffusive) of these multifunctional particles, multiple enzymes (urease and catalase), and magnetic nanoparticles. We show their potential for carrying photocatalysts and the encapsulation and release of drugs (carboplatin). Our approach provides a straightforward method for engineering functional soft microcarriers by controlling phase behavior through drop evaporation.

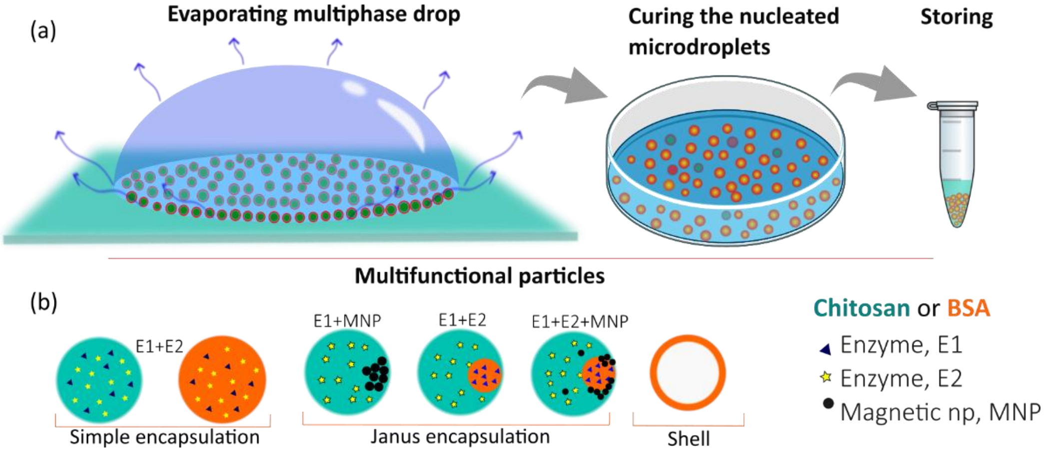

Figure 1: Functional particles via evaporative LLPS of multicomponent aqueous droplets containing (i) PEG–DEX–CS or (ii) PEG–BSA. Enzymes (E1 and E2) and magnetic particles (MNP) are simultaneously encapsulated during LLPS. The micro-condensates are subsequently cured to form stable particles and even active shells.

Edge states, pairing, and sorting of motile chiral particles

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We present experiments on chiral active polar particles, realized as vibrated granular rods, revealing the formation of robust ``skipping orbits" at hard boundaries. These edge states exhibit a net circulation opposite to the particles' intrinsic rotation and lead to a pronounced accumulation at the boundary, stronger than for their achiral counterparts. The directed nature of these orbits provides a simple yet high-fidelity mechanism for chiral sorting -- even for solitary particles, unlike in T Barois et al., Phys. Rev. Lett. **125**, 238003 (2020). We propose a unified theoretical framework for boundary interactions of both chiral and achiral particles. In this model, an effective outward radial force, proportional to motility and chirality, explains the observed boundary-hugging. Our theory predicts, and our experiments confirm, a transition in the pairing of two particles of the same chirality, from apolar spinners to polar circle walkers, with increasing packing fraction of an ambient medium of beads.

AcM+BM-Oral-38

Micelle-like clusters in swarms of self-propelled asymmetric particles

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In active matter physics, various collective phenomena in self-propelled particles with symmetric shapes have been extensively considered [1], while the formation of collective structures by asymmetric particles remains less explored.

In the present work, we study the swarms of asymmetric teardrop-shaped particles that can form micelle-like clusters by orienting their cusps towards the common point. We apply a kinetic Monte Carlo method [2] to perform extensive numerical simulations and extend our recent experimental results for the swarms of vibration-driven teardrop-shaped robots [3] placed on a flat surface or in a parabolic potential. Our findings demonstrate that the presence or absence of micelle-like clusters in the system is determined by the location of the center of inertia of robots. Moreover, we investigate how the friction coefficient between the lateral surfaces of robots, the packing density of the system, and the activity of robot motion affect the formation and stability of micelle-like structures. Finally, we show that the mechanisms that govern the formation of micelle-like clusters involve at least two-particle interactions.

The work is supported by the Russian Science Foundation (project 25-22-00768).

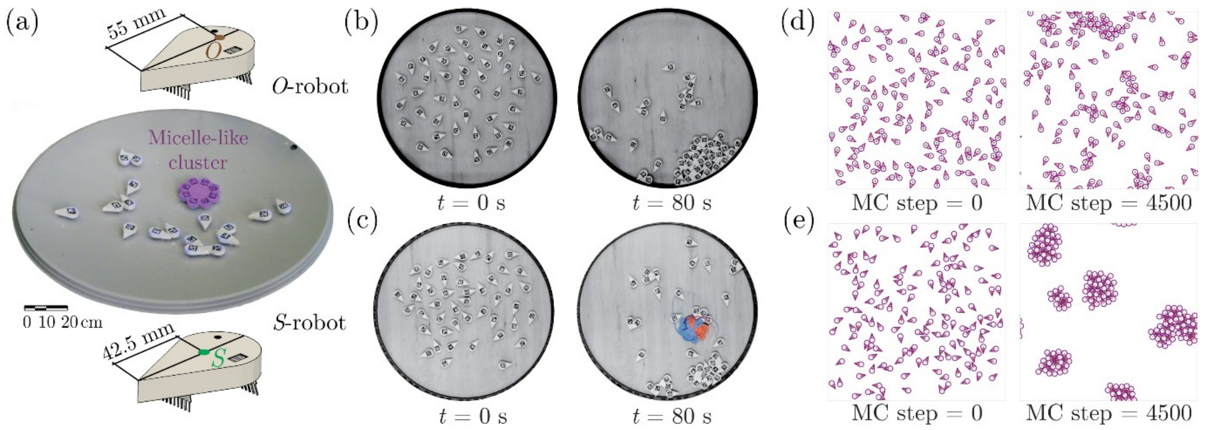

Figure 1: (a) An example of a micelle-like cluster (shaded purple) formed in the robotic swarm in a parabolic barrier. The insets show the robots with the center of inertia at point O (O-robot, top) and at point S (S-robot, bottom). (b,c) Swarms of robots moving on a flat surface for (b) O-robots (no micellization) and (c) S-robots (a micelle-like cluster is shown). (c,d) Numerical simulations of time evolution of a swarm of self-propelled particles from a random initial configuration for (d) O-particles and (e) S-particles. The labels at the bottom show the kinetic Monte Carlo simulation step number.

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[2] J. Klamser, O. Dauchot, J. Tailleur, *Phys. Rev. Lett. 127, 150602 (2021)*

[3] A. Molodtsova, M. Buzakov, O. Burmistrov, A. Rozenblit, V. Smirnov, D. Sennikova, V. Porvatov, E. Puhtina, A. Dmitriev, N. Olekhno, *Phys. Rev. E 111, 065424 (2025)*

Many-Body Systems by Self-propelled Ion Gels

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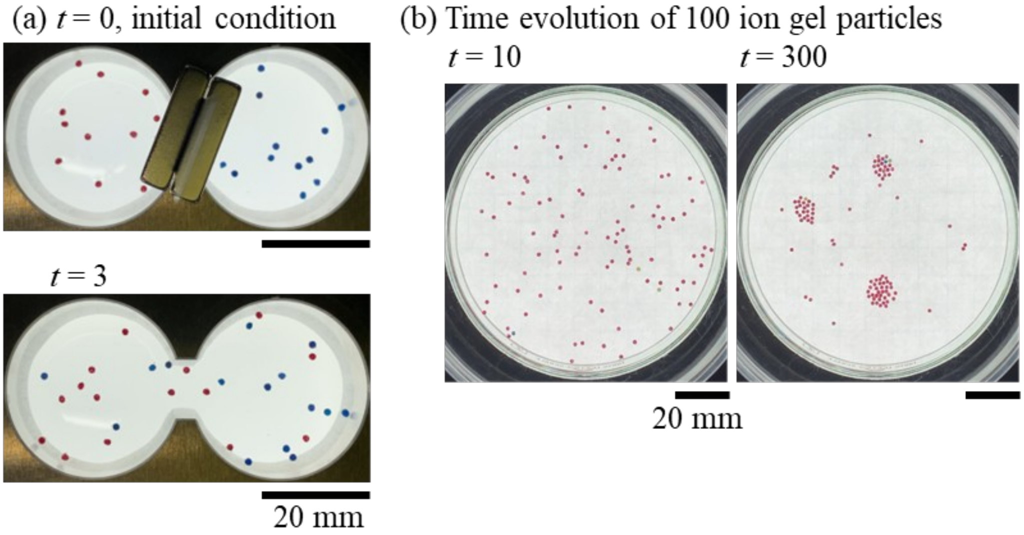
We have discovered that a specific ion gel (a gel composed of ion gel and polymer) behaves as a new type of active matter that moves spontaneously on the water surface [1]. The driving force for this autonomous motion is the surface tension gradient caused by the non-uniform dissolution of ionic liquid on the water surface. In this study, we report our recent research on phenomena observed in ion gel many-body systems (number of bodies $n = 10 \sim 100$).

Ion gel many-body systems have almost negligible interactions between gel particles. Individual particles move freely within a time domain where the self-propelled motion is sufficiently fast. Taking advantage of this characteristic, we designed an experiment that mimics the molecular kinetic theory of gases. We observed the time evolution of the motion of ion gel particles in a water chamber with two areas (Fig. 1a). Red and blue ion gels, initially introduced separately into the left and right chambers, distribute equally between the left and right within a few seconds. We discuss the statistical properties of this system.

The self-propelling force of the ion gel weakens over time, gradually decreasing its speed and eventually coming to stop. When observing an ion gel many-body system for a long period of time, there is a time region in which the cohesive force among the ion gel particles due to surface tension and the weakened self-propelling force are in opposition. We discovered that during this process, the particles form aggregates accompanied by pulsating motion (Fig. 1b). We discuss this formation process.


(a) $t = 0$, initial condition

(b) Time evolution of 100 ion gel particles

Figure 1: The ion gel many-body system we studied. (a) Experiment using a water chamber with two areas to mimic the kinetic theory of gas molecules. (b) Pulsating-aggregation formation of the many-body system over time.

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AcM+BM-Oral-40

Does chemotaxis enhance target search by active Brownian particles?

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We investigate how active Brownian particles with chemotaxis improve target search in environments with memory by dynamically forming steady paths. The particle dynamics are governed by a modified Keller-Segel model, incorporating coupling between particle orientation and a chemoattractant field generated by its own motion. We simulated several scenarios to study the cumulative effect of environmental memory and chemotaxis on particle's exploration of the accessible space and target search. The particle's behavior is sensitive to the fine balance between many parameters, including the diffusion rate, the translational and rotational chemosensitivity, and chemoattractant secretion and decay rates. We have found the narrow region of parameters at which active Brownian particles form steady channels while exploring the whole available space. Next, the joined effect of channeling and reinforcement (by a temporary chemotaxis boost) when reaching a target results in the formation of a strong "chemoattractant bridge" between the origin and the target. Consequently, it forces particles to move towards the target and reach it one order of magnitude more often than without reinforcement.

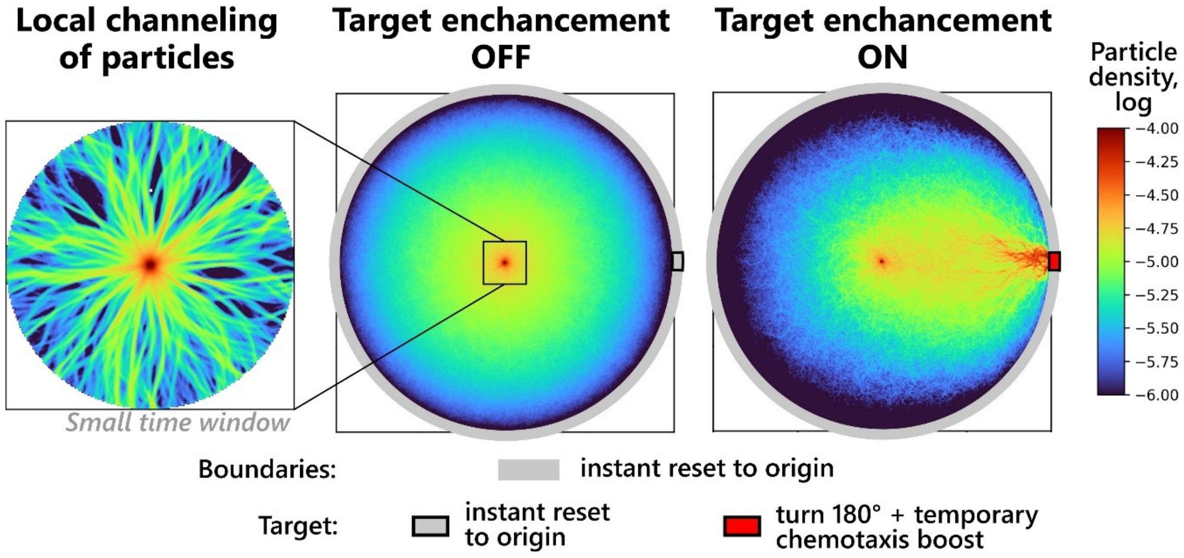

Figure 1: Particle density distributions for a small arena (left), for large arena without specific target (center), and for reinforcement of a 5 degree target (right). Target reinforcement leads to symmetry breaking towards target and increases number of target hits by one order of magnitude.

AcM+BM-Oral-41

Microfluidic Insight of Nanoparticle’s Role in Bacterial Remediation of Water: Materials to Devices

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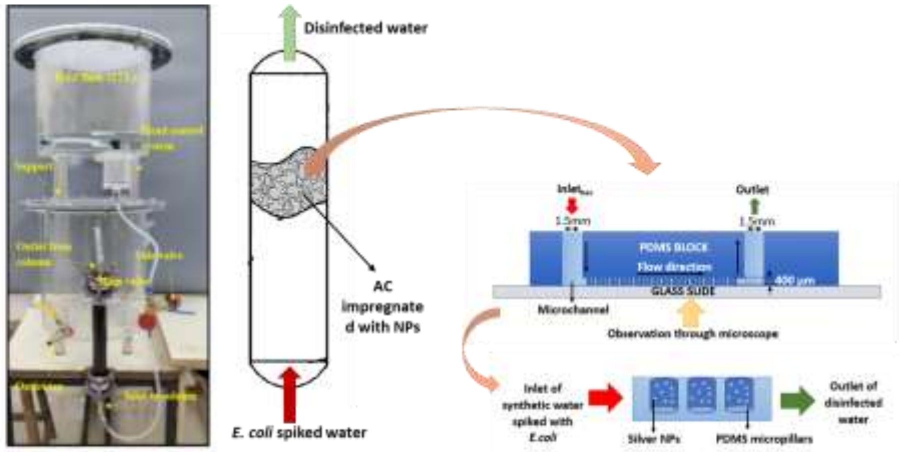
We have synthesized nanoparticle-based composites for removal of contaminants (e. g. microorganisms like *E. coli*), which is essential to have clean, potable water. For microbial remediation, it is essential to have a cheap and continuous supply of potable water, devoid of any microbes. To this end, we have synthesized silver-copper, dual nanoparticle (NP)-impregnated, porous activated carbon (AC) as a cheap, sustainable material. Substantially enhanced disinfection rate was possible, resulting in desirable higher throughput of potable water.

Subsequently, this has been translated into in-house designed, gravity-driven water disinfection devices, which run without the use of electricity or any other power source (Fig. 1). The principle of this disinfection process is based on three-phase, biotic-abiotic interaction between the static AC substrate, impregnated Ag-Cu NP and *E. coli*, the latter flowing-in with the contaminated, inlet water. Simultaneously, we also conducted experiments in our microfluidic device (Fig. 1) to mimic the intergranular-carbon pores of AC, simulating the nanoparticle-carbon-bacteria three-way contact.

We analyzed various bacterial trajectories experimentally and through simulation to infer that, although translational diffusivity is hindered due to presence of NPs, rotational diffusivity is enhanced. So, we conclude that, in order to avoid the NPs, *E. coli* undergoes a higher turning motion, within the channels of the packed AC filter-column, in order to escape the NPs. This gives us fundamental insights of this process, allowing inverse design rules to better fabricate the packed filter column, thereby driving the desirable enhanced water disinfection rate in any practical water disinfection device.



AcM+BM-Oral-41

Figure 1: Photograph of gravity-driven, field-device for water disinfection and corresponding microfluidic set-up to study role of nanoparticles in killing microbes in water.

Arrested Matter (AM)

Influence of Equilibrium and Nonequilibrium Effects on Surface Mobility in Polymer Glasses

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Using angle-resolved X–ray photoelectron spectroscopy, sum-frequency generation vibrational spectroscopy, contact angle measurements, and molecular dynamics simulations, we verify that the glass transition temperature (T_g) of polymer glass is lower near the free surface. However, the experimental T_g–gradients showed a linear variation with depth (z) from the free surface, while the simulated equilibrium T_g–gradients exhibited a double exponential z–dependence. In typical simulations, T_g is determined based on the relaxation time of the system reaching a prescribed threshold value at equilibrium. Conversely, the experiments determined T_g by observing the unfreezing of molecular mobility during heating from a kinetically arrested, non-equilibrium glassy state. To investigate the impact of nonequilibrium effects on the T_g–gradient, we reduced the thermal annealing time in simulations, allowing the system to fall out of equilibrium. We observe a decrease in the relaxation time, and the emergence of a modified z–dependence consistent with a linear T_g–gradient near the free surface. We further validate the impact of non-equilibrium effects by studying the dependence of the T_g on the heating/cooling rate for polymer films of varying thickness (h). Our experimental results reveal significant variations in the T_g–heating/cooling rate dependence with h below the bulk T_g, which are also observed in simulation when the simulated system is not equilibrated. We explain our findings by the reduction in mass density within the inner region of the system under nonequilibrium conditions, as observed in simulation, and recent research indicating a decrease in the local T_g of a polymer when placed next to a softer material. This work has been published in *The Proceedings of the National Academy of Sciences, U.S.A.* [1].

The authors would like to express their gratitude for the funding support received for their research. JX and XW were supported by the National Natural Science Foundation of China (grants 22161160317, 22203075, and 22173081). OKCT received support from the Research Grants Council of Hong Kong (grant N_HKUST623/21 and 16300824). DSS and AG were supported by the United States National Science Foundation CBET Program (grant 2208238).

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Squishy Amorphous Matter

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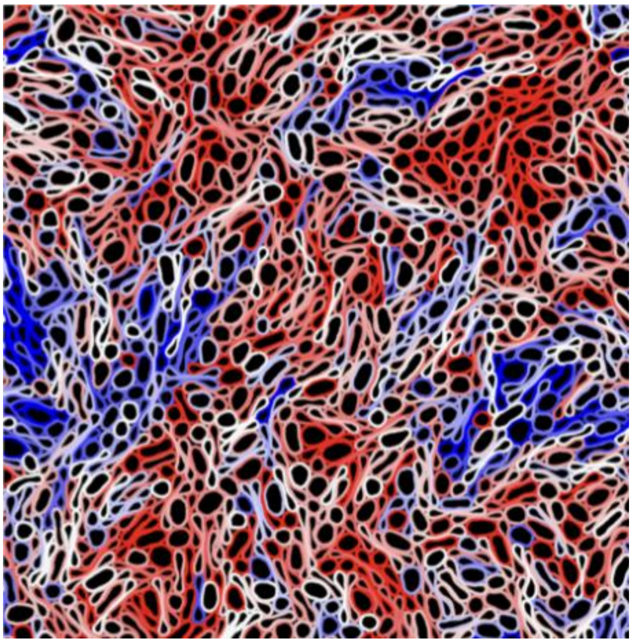
Soft glassy materials are widespread in nature and technology and often consist of deformable particles, yet the role of particle flexibility in glass formation, jamming, and mechanical response remains not well explored. Using extensive numerical simulations of two-dimensional ring-polymer assemblies as a model for such squishy amorphous materials, we examine how densification and polydispersity shape structure and, in turn, govern the dynamics. Focusing on the amorphous states that emerge upon densification, we show that relaxation dynamics and mechanical responses are closely linked to underlying structural features, highlighting the freedom to change shape as a central control knob for the observed material behavior.



How is active glass more heterogeneous?

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We compare the approach to the glassy regime of 2D passive and active mixtures as a function of area fraction. In our experiments, a bidisperse mixture of frictional discs, confined to the horizontal plane, is fluidized by vertical vibrations. These discs are designed either to be ‘passive’, that is, exhibiting isotropic motion in the plane, or ‘active’, with a preferred polar mobility. We compare dynamics in 50:50 mixtures of large active and small passive discs to 50:50 mixtures of large passive and small passive discs. At equal area fractions, the active system shows faster dynamics. The question we explore is whether activity merely speeds up the dynamics or if active and passive systems with the same relaxation time exhibit qualitatively different dynamics. The four-point correlation function shows that the heterogeneity in the active system is much larger. The active system also shows longer-ranged spatio-temporal velocity correlations, and longer-lived mobile chains. Though there are stronger velocity correlations, there are essentially no correlations between the activity direction of particles, nor is the displacement well aligned with the activity direction, thus presenting a puzzle as to how activity leads to such strong heterogeneity

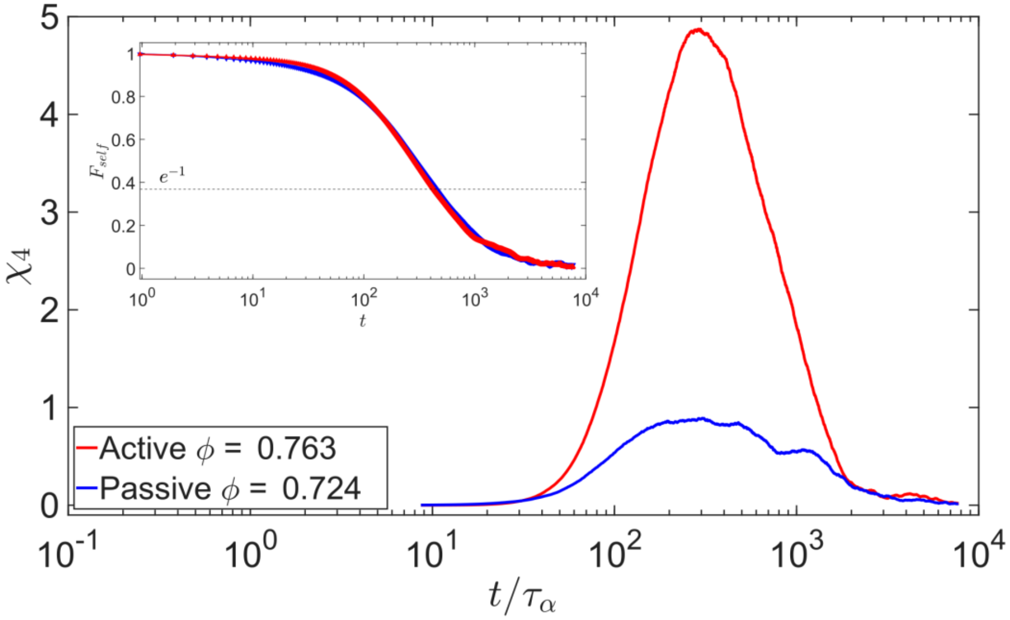

Figure 1: Comparing an active and a passive system with the same relaxation time. Inset: The self-intermediate scattering functions at the chosen area fractions are identical. Main figure: The 4-point correlator shows that the heterogeneity is much higher in the active system.

Trainable amorphous matter: tuning yielding by mechanical annealing

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Living organisms can demonstrate highly adaptable and sophisticated responses using ‘memory’ resulting from repeated exposure to external conditions aka ‘training’. However, realizing similar adaptability in mechanical responses in inanimate, physical materials presents an outstanding challenge in several fields, including soft matter, materials science, and the domain of soft robotics. Our study focuses on a disordered solid formed by a dense colloidal assembly, a model system for a range of soft disordered materials. Here, combining bulk rheological experiments, in-situ optical imaging, and numerical simulations, we demonstrate how training via cyclic shear can encode memories that tune the yield point in a unique way and over unprecedented ranges. Our study reveals that such tunability is intricately linked to the plasticity–non-affine deformations, and formation of shear bands. Our numerical simulations illustrate that systems with identical internal energies, prepared via different protocols (mechanical or thermal), can display markedly different rheological responses, indicating that internal energy alone does not determine mechanical behaviour. Moreover, while the yield strain increases with training amplitude, the material simultaneously softens, contrasting with the thermal case, where both quantities increase monotonically with increasing degree of annealing. Our results establish mechanical training as a powerful strategy to design trainable amorphous matter, opening up new possibilities to access the material-feature space far beyond those achievable through thermal annealing alone.

[1] M. Mandal *et al.*, arXiv:2512.01019 *(2025)*

Stabilization of co-amorphous mixtures via T_g elevation driven by molecular interactions

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Co-amorphous drug mixtures (CAMs) (i.e., co-amorphous glasses) have the potential to enhance the oral absorption of poorly soluble drugs but also suffer from stability issues associated with the amorphous phase. Enhancing the glass transition temperature (T_g) of CAMs can improve their physical stability against crystallization and extend shelf life during storage. In this work, we establish a generalized design framework (**Figure 1**) that reveals the role of specific intermolecular interactions leading to significantly elevated T_g values and improved stability in CAMs. CAMs prepared with drugs containing the -COOH group exhibit significant positive deviations from T_g values predicted by the Gordon−Taylor equation. -COOH-associated hydrogen bonding is a key factor for T_g elevation, while π−π and halogen bonding provide synergistic contributions. Continuity in T_g as a function of varying molar ratios indicates that stoichiometric pairing has a relatively minor contribution, while a decrease in the width of glass transition suggests enhancement of molecular cooperativity as a possible stabilization mechanism. In contrast, other interactions do not promote T_g deviations on their own. Stability studies indicate that CAMs exhibiting high T_g elevation and specific interactions are more stable against isothermal crystallization at temperatures well above T_g, despite possessing higher mobility and fragility. Systematic correlations between T_g deviations and molecular interactions, as well as their influence on CAM crystallization tendency reported in this work, can lead to generalized rules for the design of stable co-amorphous glasses.

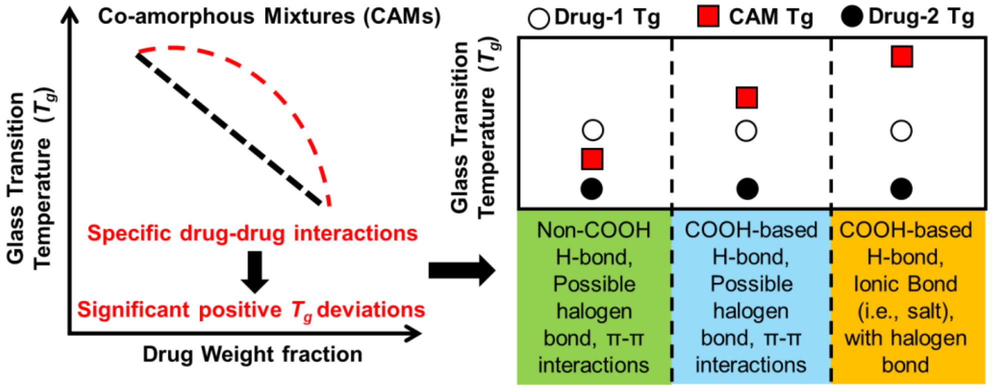

Figure 1: Intermolecular interactions that lead to elevation in T_g and CAM stability

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Granular materials from soft inflatable particles

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The mechanical properties of granular packings are closely tied to particle configurations and the interparticle interactions within the system. Particle-level changes, such as packing arrangement, as well as particle properties including surface friction and deformability, can significantly alter macroscopic behavior, influencing phenomena such as the onset of rigidity and the effective material moduli. To investigate these effects, we have developed inflatable particles with tunable control over the size and stiffness of individual grains. We have created a two-dimensional packing platform composed of inflatable particles that allows continuous tuning of packing parameters while directly monitoring the system's mechanical response. Our goal is to identify governing rules that link particle-level properties to bulk mechanical behavior and to use these rules to predictably modify the response of granular packings. Ultimately, this work provides a pathway toward creating trainable granular metamaterials that can be evolved through local feedback.

Two-step Devitrification of a Soft Colloidal Glass

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Understanding devitrification, the transformation of a glass to crystal, is crucial to ensure glass stability. However, direct experimental observation of this phenomenon at the particle level has remained scarce owing to its stochastic nature, leaving its microscopic pathway poorly understood. Here we investigate devitrification in a soft colloidal glass using single-particle resolved confocal imaging, combined with a four-point correlation analysis that captures structural order beyond the nearest-neighbour shell. Our analysis reveals that angular correlations emerge at the intermediate range before the onset of translational order, revealing a two-step process. In addition, these angular correlations already encode the symmetries consistent with the final crystalline state. Our results suggest that intermediate-range angular correlations represent the earliest structural signatures of devitrification.

Models of yielding and fatigue failure under cyclic shear deformation of glasses

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The phenomena associated with yielding and elasto-plastic flow in amorphous solids have been extensively investigated through computer simulations [1] and through theoretical investigations of theoretical models [2], including the so-called elasto-plastic models [3]. In particular, plasticity and yielding under cyclic shear deformation have received significant attention. An important phenomenon in solids subjected to cyclic deformation or stress is that of fatigue failure, which occurs after a number of cycles, with the number of cycles to failure exhibiting a divergence as the yield point is approached. We will discuss our investigations of these phenomena using an elasto-plastic model that has been developed based on an energy landscape picture, and using finite element modeling [3]. Such a model captures many features that are observed in simulations, but also reveals several key aspects involved in the modeling that are not well understood. Results illustrating both the successes and limitations of the model are presented. The elasto-plastic model is also employed to elucidate key aspects of theoretical approaches [2] to the fatigure failure phenomenon.

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[3] P. Khandare, S. Sastry (To be submitted)

Local structural measurements of glasses from small-beam diffraction

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Small-beam diffraction measurements such as micro-small angle x-ray scattering (μSAXS[1]) and electron nanodiffraction (END[2]) are promising methodologies to probe local structure in glasses, ranging from colloidal assemblies made from microparticles to metallic glasses composed of atoms. In this scattering geometry, you obtain "speckle" diffraction patterns that contain an intensity distribution that reflects the local order in the volume being probed[3]. The information in these patterns is extremely rich and can be used to quantify local order in glasses[1,4] and spatially resolve structural and dynamical heterogeneity[5]. More recently, we have been examining local centrosymmetry and strain (dilation/contraction and anisotropy) in nearest-neighbour configurations to pinpoint the particle-level structural transformations that mediate deformation – or 'defects'[5,6]. Scanning, small, coherent beam diffraction is a versatile experimental platform to provide the missing connections between local structure in glasses and their global behaviours and properties.

The authors acknowledge the use of the instruments at the Monash Centre for Electron Microscopy, a Microscopy Australia (ROR: 042mm0k03) facility supported by NCRIS, and equipment funded by the Australian Research Council (ARC LE045416, LE200100132). This research was undertaken on the SAXS/WAXS beamline at the Australian Synchrotron, Victoria, Australia. ACYL/TP acknowledge support from the ARC (FT180100594, DP250102966).

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[3] ACY Liu, GR Lumpkin, TC Petersen, J Etheridge and L Bourgeois, *Acta Cryst. A*, (2015) **71**, 473–482.
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Probing Anharmonic and Heterogeneous Carrier Dynamics Across Sublattice Melting in a Minimal Model Superionic Conductor

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Despite decades of research, the microscopic origin of sublattice melting and fast ion transport in superionic conductors remains elusive. Here, we introduce a minimal binary model that captures these essential features without invoking any chemically specific interactions. The system consists of two coexisting crystalline components: a rigid host lattice stabilized by short-range steric repulsion and a soft carrier sublattice interacting through long-range, Wigner–type forces. This physical contrast naturally yields distinct melting temperatures for the two sublattices, leading to the spontaneous emergence of a sublattice-melting phase in which carriers become fluidlike [1]. At the same time, the host lattice preserves crystalline order. Systematic molecular-dynamics simulations reveal three dynamical regimes—crystalline, sublattice-melt, and fully molten—characterized by sharp changes in diffusivity, structural correlations, and dynamic heterogeneity. The carrier sublattice exhibits strongly anharmonic and spatially heterogeneous dynamics that cannot be captured by mean-field hopping descriptions, indicating that collective fluctuations and lattice anharmonicity play a decisive role in enabling rapid ion motion. By tuning the density, we demonstrate that the extent and sharpness of sublattice melting can be continuously controlled, establishing a direct link between lattice softness, anharmonicity, and ionic transport. This framework clarifies how collective interactions drive sublattice melting and guides the design of robust, high-performance superionic conductors.

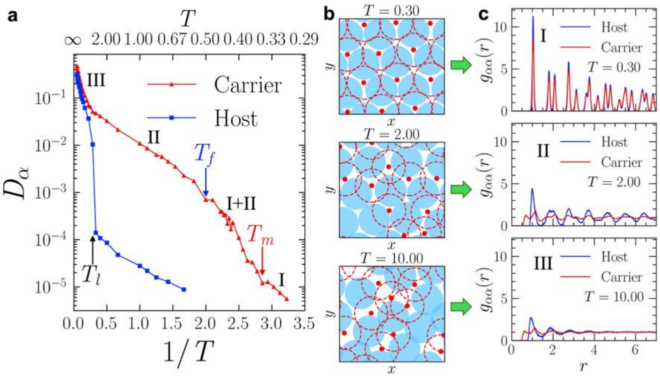

Figure 1: **Selective sublattice melting across temperature:** (a) Diffusivity (D) vs. inverse temperature ($1/T$) showing crystalline (I), sublattice-melted (II), and fully melted regimes (III); (b) corresponding structural snapshots; (c) the radial distribution function $g(\mathrm{r})$ revealing coexistence of mobile carriers and ordered host lattice.

[1] J. Ding, M. K. Gupta, C. Rosenbach et al., *Nat. Phys. 21, 118-125 (2025).*

From Disorder to Discovery: Bridging Glass Physics and Machine Learning for Predictive Materials Design

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ABSTRACT

Glasses represent one of the most fascinating yet enigmatic classes of materials, where structural disorder gives rise to remarkable physics and diverse functionalities. A key challenge is understanding why seemingly similar disordered environments of glass microstructure can lead to very different properties. This question is not only fundamental but also central to designing glasses with tailored performance. In this talk, I will trace the journey from the physics of glass formation to the development of machine learning models [1,2] that predict glass properties. I will conclude by discussing possible extensions of these models and how insights from glass physics can enhance the predictive power of ML approaches for materials design [3,4].

Keywords: Glass, Disorder system, Machine Learning, Molecular Dynamics Simulation

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Geometrical Fingerprints of Stability in Binary Colloidal Glasses

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The microscopic structure of a glass corresponding to a configuration in the underlying energy landscape governs its thermodynamic stability as well as its kinetic and mechanical response to external perturbations. In practice, however, stability is most often assessed indirectly through dynamical measurements under applied perturbations, rather than inferred directly from static structure. This is because conventional two-point structural correlators are insufficient to reliably distinguish among metastable glassy states. However, whether static many-body structural descriptors beyond pair correlations can uniquely encode metastable states and their stability remains an open question. Here, we investigate microscopic structural quantifiers pertaining to stability in binary colloidal glasses using a combination of experiments, simulations, and machine learning. We first identify plausible candidate geometrical features, such as Voronoi and hexatic order parameter based measurements, that might correlate with the stability of a glassy state. Next, we construct a machine learning-based higher-order structural encoder and utilize it to rank the fidelity of these geometrical descriptors. Remarkably, we can mathematically tune this structural encoder to discern between the stabilizing versus destabilizing effects of single-particle perturbations with high fidelity. In total, our findings reveal that the physical information governing the depth of a glassy state is geometrically encoded in the raw particle coordinates albeit in a non-linear fashion, providing a pathway to predict the relative depth of inherent states of glasses without the need for exhaustive dynamic sampling in both simulations and experiments.

Aging in Amorphous Solids under the Influence of Soft-Pinning Particles

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The dynamics of aging aqueous colloidal Laponite suspensions (a model glass former) with dispersed polystyrene (PS) particles, used as soft pinning sites, were studied. The included PS particles, being larger and less mobile than the Laponite particles, are expected to diffuse very slowly and act as nearly pinned particles. Intensity-intensity autocorrelation functions, measured in dynamic light scattering experiments, show the existence of a two-step relaxation process in these suspensions. The fragility parameter was calculated with increasing concentration and sizes of the included PS particles. As the concentration of polystyrene (PS) particles was increased, the aging dynamics of Laponite was observed to slow down. In contrast, increasing the sizes of the PS particles accelerated the aging dynamics. Furthermore, the growth of amorphous order in the presence of soft-pinned particles was estimated by calculating pinning length scales. It was found that the pinning length scales were highest when the pinned particles were largest. We next simulated glass-forming liquids with larger, heavier particles serving as soft-pinning sites and reproduced the experimental observations. Our work demonstrates that the fragility of a colloidal glass former can be tuned by changing the sizes of soft-pinned particles.

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Colloids (C)

C-Keynote-01

High-precision measurements of colloidal interactions using holographic microscopy

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Measurements of interactions are crucial to understanding the stability, structure, and dynamics of colloidal dispersions. It is difficult to directly measure these interactions for two main reasons: (1) they are typically short-ranged, operating over distances a fraction of the particle diameter; and (2) the measurement technique can often perturb the interaction. I will discuss how holographic microscopy can be used to measure colloidal interactions non-invasively and with high precision. An important part of the measurement is inferring the interaction from the experimentally recorded holograms. To do this, we use a Bayesian framework to fit scattering and dynamical models to the data. I will discuss how we use this approach to measure particle-particle potentials and interactions between a particle and a liquid interface.

C-Keynote-02

Photoreactive Pluronics: Tailoring Self Assembly Through UV Induced Crosslinking

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Pluronics are amphiphilic block copolymers that self-assemble into a wide range of microstructures in water, with their morphology strongly dictated by temperature. This structural landscape can be further tuned through additives such as salts or acids. Among them, Pluronic F68 is notable for forming micelles and body-centered cubic (BCC) crystalline phases under specific thermal and concentration conditions. These transitions are fully thermoreversible - an advantage for material recovery and reuse, yet a drawback for biomedical contexts where stability is required in highly hydrated environments.

To overcome this limitation, we designed UV-responsive Pluronic derivatives by incorporating photo-sensitive groups at the molecular level, enabling controlled crosslinking upon irradiation. The chemo-rheological evolution of these modified systems under UV light was characterized using an Anton Paar MCR 702 rheometer equipped with a transparent Peltier plate and UV source, operating within the linear viscoelastic regime. Time-sweep experiments were performed across multiple temperatures and polymer concentrations, while maintaining a constant radical initiator level.

The resulting crosslinked systems - whose mechanical and structural properties could be precisely tuned through formulation - serve as versatile platforms for advanced technologies, including temperature-responsive sensors, soft conductive interfaces, and optical fibers for bio-interfacing.

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C-Keynote-03

Equilibrium and Non-equilibrium Melting of Colloidal Wigner Crystals on Curved Manifolds

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Monodisperse assemblies of charged colloids, adsorbed at oil-water interfaces due to image-charge forces, readily form classical Wigner crystals at suitable densities and are an elegant experimental system to study how the topology of the host surface influences the physics of condensed phases. When confined to planar interfaces, these crystals melt via an intermediate hexatic phase – a seminal prediction of the celebrated Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young (BKTHNY) theory of two-dimensional melting. However, the mechanism(s) by which crystals draped on non-Euclidean surfaces melt remain unexplored. In my talk, I will present results from particle-resolved experiments probing the melting dynamics of colloidal Wigner crystals on curved surfaces with Gaussian curvature (κ), spanning from negative (catenoids) to zero (cones and cylinders) to positive (spheres and barrels). We show for the first time that Gaussian curvature fundamentally alters the melting mechanism: both equilibrium and non-equilibrium melting on surfaces with $\kappa \geq 0$ follow the BKTHNY scenario, whereas for $\kappa \leq 0$, we observe single-step melting. We rationalize our results using analytical calculations that show that the Gaussian curvature alters the defect unbinding dynamics and directly influences the nature of the melting transition.

Microemulsions As Confined Reaction Media For The Synthesis Of Metalic Nanostructures And Nanomofs

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Since first reported in 1982[1] the microemulsion reaction method has been employed extensively for synthesis of a variety of metallic, metal oxide and other inorganic nanoparticles with a narrow size distribution, high specific surface area and a good performance in certain applications such as catalysis. Most of those investigations were based on water-in-oil (w/o) microemulsions. However, the use of w/o microemulsions requires high amounts of solvent, hindering its applications at the industrial scale. Hence, from a practical point of view, the possibility of using oil-in-water (o/w) microemulsions may offer advantages, since the major phase is water. Such approach implies the use of organometallic precursors, dissolved in nanometer scale oil droplets (stabilized by surfactant), and dispersed in the continuous aqueous phase; the precipitating agents, can be added directly as aqueous solutions. It was reported for the first time as a proof of concept by our group in 2009 [2]. On the other hand, in recent years we also investigated the synthesis of inorganic nanomaterials in nonionic bicontinuous microemulsions, resulting in hierarchical superstructures of metal, metal oxide and some hybrid systems, such as Pt nanocorals used as electrocatalysts[3]. Our latest efforts are being directed towards the synthesis of nanostructured MOFs in W/O, O/W and bicontinuous microemulsions, and we have been able to obtain some nanostructured MOFs of the UiO-66 family at room temperature. UiO-66-NH_2 NPs were obtained both in O/W (20-40 nm) and W/O (10-20 nm) microemulsions; curcumin was successfully loaded in these systems. UiO-66-F_4 nanoflowers and nanosponges were obtained in O/W and bicontinuous microemulsions, respectively. These systems were loaded with plasmonic nanoparticles which were used successfully for the detection of PFAS (perfluorooctanoic acid), reaching a detection limit of 0.4 ppt. The obtained results demonstrate the feasibility of this approach for the preparation of a great variety of nanomaterials including nanoMOFs with many potential applications, in particular those related with electrocatalysis, SERS substrates and drug delivery.

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C-Keynote-05

Soft modes in strain softening composite colloidal networks

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Soft composite materials commonly display strain softening and stiffening under large deformation, which is often accompanied by hysteresis from progressive microstructural damage or incipient failure. Here, we investigate the microscopic origins of these strain-dependent transitions in soft biopolymer hydrogels composed of a strain-stiffening agarose matrix, reinforced by a ductile and strain-softening network of colloidal chitosan microfibers. A sol-gel transition occurs when the agarose is cooled below the gel point, during which the chitosan nanocolloids self-assemble into a complex architecture within the agarose. Both networks have opposing deformation modes and are fluorescently tagged to enable in situ direct visualization during rheological measurements. The presence of soft chitosan networks results in a complex stiffening-to-softening transition of the composite material in response to various oscillatory and steady shear strains, along with a substantial increase in linear stiffness relative to pure agarose. Confocal rheology shows that the applied stress is distributed such that the microfibrous chitosan fillers undergo reversible hinge-like unbending prior to the permanent lengthening of the bulk agarose network. The unbending motion accommodates the applied deformation by disspiating bending stress without causing permanent changes in either network. In contrast, strain stiffening coincides with the irreversible stretching and breakdown of agarose fibers, followed by crack nucleation and brittle fracture within the primary network. The secondary chitosan network remains intact even after fracture of the agarose matrix, suggesting that failure is initiated primarily within the primary network despite the presence of soft reinforcing fillers. These observations reveal a distinct separation between reversible softening and irreversible stiffening and suggests that unbending of the filler network serves to dissipate the externally imposed stretching energy. The results suggest a sequential load-transfer mechanism in which a ductile secondary network shields a brittle primary network from irreversible plastic deformation at intermediate strains, and delays the onset of catastrophic failure. This work provides a basis for understanding the mechanism of a class of soft composites that can stiffen without sacrificing deformability or prematurely triggering fracture.

Effect of hydrodynamic interactions in concentrated colloidal suspensions and gels: a comparative DPD and SD simulations study

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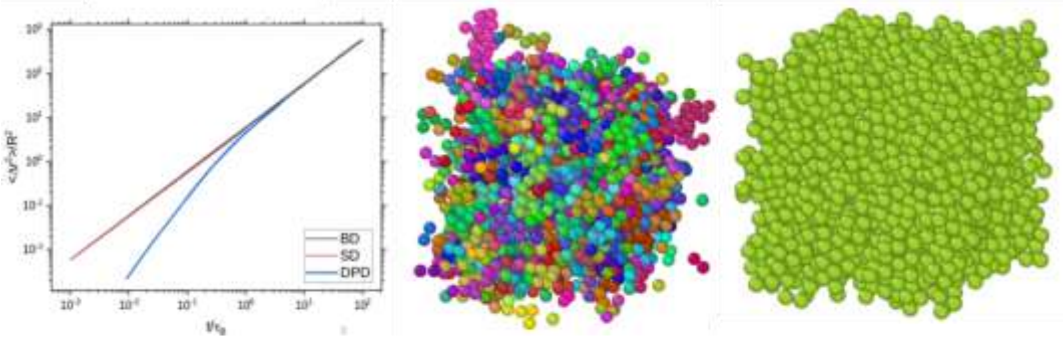
Dissipative Particle Dynamics (DPD) is a mesoscale simulation technique widely used for modeling complex fluids and soft matter systems. DPD allows for the efficient simulation of larger length and time scales by grouping atoms into coarse-grained particles. This makes it particularly suitable for studying systems such as colloidal suspensions, where hydrodynamic interactions and thermal fluctuations play a crucial role. We employed a dissipative particle dynamics (DPD) simulation method to investigate hydrodynamic interactions in colloidal systems. We explored different volume fractions, including liquid, glass, and gel states, in both attractive and repulsive systems. Additionally, we compared our simulation results with other established methods such as Brownian Dynamics (BD), Stokesian Dynamics (SD) and Dissipative Particle Dynamics (DPD) to assess accuracy and consistency. Furthermore, we examined the behavior of these systems under shear flow, providing insights into their rheological properties. The volume fractions (φ) used in this study were around 30%-45 % and strength/range of attraction were around 20kT/10%. Additionally, the origin of experimentally observed yield behaviour, such as 2 vs 1 step yielding, was probed computationally. We found a set of parameter values in DPD which produced a good agreement in dynamic properties such as mean square displacement (MSD) at long time, with SD and BD simulations (Fig. 1A). Additionally, we quantified network formation via cluster analysis of colloidal particles during gelation (Figs. 1B and C)



A B C

Figure 1: Mean squared displacement of colloidal particles acting like hard spheres, φ=0.01 (A). Network formation of colloidal particles, φ=0.44, in DPD simulations, shown by snapshots before (B) and after gelation (C) via cluster analysis where particles are colored according to their cluster id.[1]

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[1] Work in collaboration with Safa Jamali (Northeastern University), Dimos Aslanis and Joost de Graaf (Utrecht University)

Towards Demystifying the Odyssey of Ouzo in Polymer Nanoprecipitation

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Nanoprecipitation is an established method for producing lipid and polymer-based nanocarriers and has been central to the largescale production of mRNA loaded lipid nanoparticles used in COVID-19 vaccines. Instantaneous generation of small droplets with a narrow unimodal size distribution (50–300 nm) by solvent-shifting, requiring no mechanical energy input, surfactants, or chemical reaction, leverages on the spontaneous emulsification process known as the Ouzo effect, named after the Greek beverage. Although the Ouzo phenomenon is well characterized in ternary oil systems,[1] significantly fewer studies have examined polymer–solvent–antisolvent systems. Deciphering the factors that control the location of the Ouzo boundary is central to understanding polymer particle formation mechanisms via nanoprecipitation and eventual control of their physico-chemical properties.

Our study presents a comprehensive investigation of factors such as polymer molecular weight, solvent, surfactant and mixing on the location of the Ouzo boundary by employing complementary characterization techniques such as visual observation, optical density, dynamic light scattering and electron microscopy. The binodal line was determined by monitoring change of transmittance as water was added to PLGA (Poly (Lactic-co-glycolic) acid) solutions in THF (tetrahydrofuran). Thereafter, polymer mass fractions for nanoprecipitation studies were chosen well below the binodal line. At constant solvent fraction, increasing polymer mass fraction resulted in a progression from unimodal particle size distributions to distributions exhibiting a shoulder, then to distinctly bimodal profiles with two well separated peaks; at even higher polymer fractions, the appearance of gels or flakes indicated that the system had exceeded the thermodynamic stability limit.

Our findings show that both polymer molecular weight and solvent choice substantially shift the Ouzo domain toward higher polymer mass fractions, whereas the presence of nonionic surfactant Tween 80 in the aqueous stream affects only hydrodynamic particle size without appreciably altering the boundary. At higher molecular weight of PLGA (24-38 kDa), mixing mode (batch, semi-batch or continuous mixing timescales varying from several s to ~2.5 ms respectively) did not significantly change the boundary location, although continuous mixing yielded results consistent with previously reported Ouzo stability limits in semi batch nanoprecipitation, despite the use of different surfactants [2]. Collectively, these observations provide essential groundwork for a mechanistic understanding of nanoparticle formation in polymer nanoprecipitation systems.

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C-Oral-03

Light-Directed Colloidal Assembly

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Controlled assembly and patterning of micro-/nanoparticles have attracted significant attention because of its potential applications in various domains, including photonic devices, electronic devices, sensors, and catalysis, to mention a few [1-2]. The conventional patterning techniques rely on top-down approaches such as photolithography, ion beam lithography, and electron beam lithography [3-4], where sophisticated/expensive instrumentation, master structures, and specific masks are required. Bottom-up approaches are emerging as an alternative, as they are easy to implement, inexpensive, and provide high throughput [5]. Among them, light-controlled patterning techniques are particularly interesting as they offer real-time, programmable, and non-contact control over the patterning process [6-8]. Exploiting optically controlled fluid flow has proven effective for the assembly/patterning of various types of microscale and nanoscale entities at solid surfaces and fluid-fluid interfaces [7-9]. Here we focus on utilising optically controlled thermocapillary flows for the directed assembly and patterning of colloidal particles at solid surfaces. First, we will demonstrate the synergy of light-induced Marangoni flow and the vertical lifting process for the dynamic control over the three-dimensional morphology of the deposited patterns [10,11]. The localized laser illumination at the three-phase contact line (TPCL) generates a temperature gradient due to the plasmonic absorption of dispersed gold nanoparticles and thereby, a thermocapillary flow, which drives the particles toward the irradiated region, as shown in Figure 1(a). Combined with controlled substrate lifting, this enables continuous pattern formation (Figure 1(b)). Various patterns, such as continuous or intermittent lines, patterns with continuously varying widths, cross patterns, etc., are successfully inscribed. Further, the TPCL was lifted at an optimal speed under a temperature gradient that persists throughout the TPCL, resulting in a particle pattern resembling a remora disc or fishbone structure (Figure 1(c)).

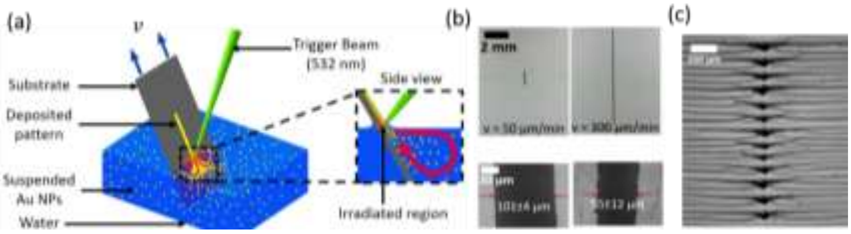

Figure 1: (a) Schematic of the plasmonically driven thermocapillary flow-based patterning of gold nanoparticles. (b) Low and high magnification images of the line pattern at different lifting velocities (v). (c) Microscopic image of the obtained remora disc pattern.

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Instabilities in Dried Colloidal Films: Role of Particle Concentration, surface charge, Substrate Wettability, and Solvent

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The evaporation of complex fluids, such as colloidal dispersions, polymer solutions, and biological fluids, involves the irreversible removal of solvent, leading to complex deposition patterns. The drying of colloidal dispersions that form particulate films on substrates often results in mechanical defects, such as buckling, wrinkling, cracking, warping, or delamination.

At a fundamental level, these instabilities arise from the release of excess strain energy accumulated during particle consolidation as the solvent evaporates. We experimentally investigated the coupled effect of particle concentration, surface charge, and substrate wettability on the morphology of the colloidal film and subsequent instabilities, such as cracking and delamination in the dried colloidal film. The representative results are shown in Figures 1(a) and (b). We further examine the role of solvent composition in governing drying-induced instabilities. Figure 1(c) illustrates the tempo- ral evolution of cracking followed by delamination in a drying particle-laden water–ethanol droplet, demonstrating that, for a fixed particle loading, increasing the ethanol fraction leads to abrupt film failure. Moreover, for a fixed ethanol composition, the extent of delamination is significantly larger at higher particle loadings, as shown in Figure 1(d). Together, these results provide a systematic framework for understanding drying-induced instabilities in multicomponent, particle-laden systems, with direct implications for coatings, printing technologies, and the fabrication of functional materials.

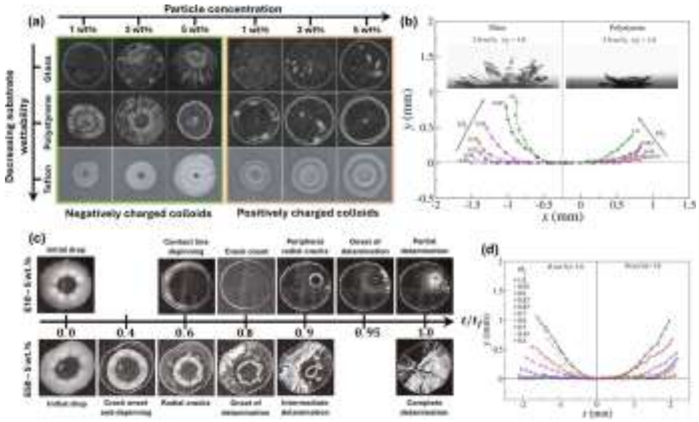

Figure 1: **Instabilities in drying colloidal films.** (a) Final dried-deposit morphologies exhibiting cracking or buckling as a function of particle surface charge, particle loading, and substrate wettability. (b) Comparison of the extent of delamination at fixed particle loading shows larger delamination on hydrophilic glass substrates than on neutrally wetting polystyrene substrates. (c) Temporal evolution of solvent- induced (ethanol) cracking and warping instabilities on a glass substrate for a fixed particle loading. (d) Effect of particle concentration on the kinetics of delamination for a 1:1 ethanol–water droplet.

Integrated DFT, Docking, and Molecular Dynamics investigation of Potent Biomolecular Complexes for Prostate Cancer Therapy

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Prostate cancer is the world's second most frequent type of malignant tumor and a leading cause of death among elderly males. Current treatment for prostate cancer focuses on drug therapy, chemotherapy, radiotherapy, and endocrine therapy; however, due to poor efficacy and drug resistance, the existing treatments are not sufficient to cure the disease. Recently combined therapies have gained momentum as an efficient treatment modality to prevent or treat cancer disease and extend patient's lifespan [1]. In this work, two biomolecular complexes are chosen to elucidate the mechanism of interaction between the amino acid L-Phenylalanine (L-Phe) and the purine base Guanine, and between DL-Phenylalanine and adenine, as a potent inhibitor of prostate cancer. Dispersion-Corrected Density Functional Theory (DFT-D3) methods were employed to examine molecular interactions and reactivity characteristics, such as the electrostatic potential, energy band gap, and density of states. Molecular docking against CDK2 protein (4EK3) and androgen receptor proteins (3rlj) depicts that Glu81 (2.66 Å), Lys33 (2.11 Å), Asp145 (2.67 Å), Asn132 (1.70 Å, 2.23 Å) residues strongly take part in the binding interaction, revealing its novel inhibition against prostate cancer. The molecular dynamics simulation indicates that the protein–ligand complex is relatively stable [3].

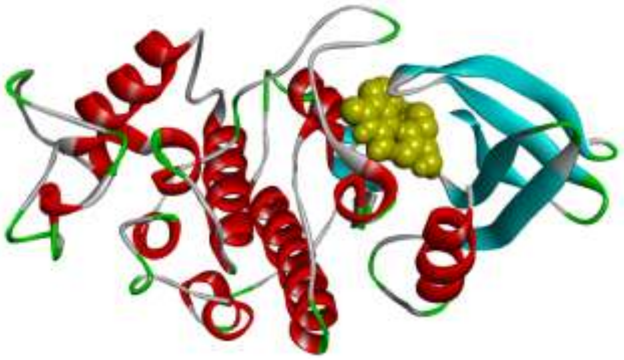

Figure 1: 3D representation of H-Bond's donor-acceptor region for L-Phe+Guanine against 1e3g protein receptor

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C-Oral-06

Aggregation mechanism in DNA functionalized gold nanoparticles in multivalent and ionic liquid environment

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The stability of colloidal nanoparticle systems is highly sensitive to both the type and concentration of salt, influencing their electrostatic interactions and surface properties. As ionic strength increases, the electrical double layer around the nanoparticle’s compresses, diminishing electrostatic repulsion. This screening effect allows dominance of attractive van der Waals forces, often resulting in nanoparticle aggregation. The degree of this destabilization depends on the specific salt, its concentration, and the nanoparticles' surface ligands.

In this study, we show that increasing ionic strengths of divalent salts and ionic liquids can induce the aggregation of DNA-coated gold nanoparticles in aqueous solution. Furthermore, we demonstrate that this aggregation behavior is strongly influenced by both the salt type and the DNA structure. Through systematic investigations using dynamic light scattering, UV-Visible absorption spectroscopy, transmission electron microscopy, small-angle X-ray scattering, and fluorescence spectroscopy, we have characterized the underlying aggregation mechanism. In the presence of divalent salts, we observed that aggregation is primarily driven by electrostatic screening and ionic bridging, leading to the formation of dense, three-dimensional aggregates at higher ionic strengths, whereas in Ionic Liquid environments, groove binding interactions play a dominant role. For double-stranded DNA, groove binding of the alkyl chains in the ionic liquid promoted robust, multi-layered aggregation, whereas for single-stranded DNA, only weak interparticle aggregation was observed. Our study highlights the importance of salt ionic strength and surface ligands on colloidal stability, offering valuable insights for tuning nanoparticle behaviour in applications such as biomedicine, catalysis, and materials science.

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Effective interactions of star-like microgels

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Soft colloids provide a unique route to tunable softness. In particular, star-like thermoresponsive microgels synthesized with a fast crosslinking agent have recently emerged as a new platform in this direction [2], combining microgel-like responsivity with a star-polymer–like internal structure. Building on our earlier structural characterization, we focus on the effective interactions [1].

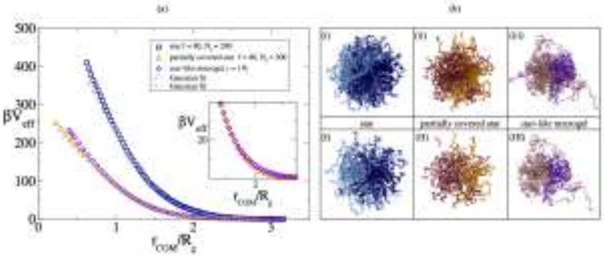

Figure 1: (a) Effective interactions for star-like microgels and star polymers, with fixed size of the core and full coverage (γ = 1, f = 80) or partial coverage fraction (γ = 0.57, f = 46). The natural variable is the distance r_{COM} between the centers of masses, normalized by the particle gyration radius R_g. (b) Snapshots for corresponding particles at close separation to highlight core coverage effects (with colored core/crosslinker-rich regions).

We perform extensive monomer-resolved simulations and directly compute the effective pair potential between star-like microgels, comparing it to standard microgels at the same crosslinker concentration and to archetypal star-polymer models. We find that the star-like microgels exhibit an effective interaction that is Gaussian over most probed distances, in sharp contrast with the Hertzian-like response of regular microgels. The repulsion is weaker than for ideal stars, and we show that this discrepancy is quantitatively captured by a star polymer with a partially covered finite-size core, pointing to core-coverage as a control parameter for softness in such architectures, and providing a basis to investigate higher–crosslinker-content star-like microgels with larger cores.

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C-Oral-08

Diffusio-Osmotic And Phoretic Transport In Ordered And Disordered Porous Media

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Chemically induced gradients are widely employed to enhance particle transport in ordered and disordered porous media. Diffusiophoresis (DP) and diffusioosmosis (DO) govern the movement of particles and near-surface fluid in response to electrolyte gradients. These transport mechanisms play a crucial role in the transport of particles and drugs in porous biofilms. Porous media contain both dead-end pores (DEP) and transmitting pores (TP), making it essential to understand particle withdrawal dynamics under different solute gradient modes: solute-out (solute-emptying pore) and solute-in (solute-saturating pore), which remain largely unexplored. This study demonstrates the impact of solute gradient orientation on the osmotic and phoretic transport of colloids withdrawn in ordered and disordered porous media. We have found that these two modes (solute-out and solute-in) exhibit different qualitative performances for colloidal transport. The two kinds of pores (DEP and TP) are also shown to be significantly different in qualitative insights for colloidal withdrawal induced by both solute gradient modes. The analytical and numerical models highlight fundamental differences between solute-out and solute-in gradient generation in ordered and disordered porous media. Beyond revealing the sensitivity of osmotic transport in porous media, insights from this study can inform alternative approaches for membrane filtration and enhance oil recovery.

Keywords: Diffusioosmosis, Diffusiophoresis, Electrolytes, Porous media.

C-Oral-09

Engineering Pickering Emulsions via Droplet Bridging by In Situ Particle Surface Modification

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The emulsions with a large interfacial area deprived of particles can be stabilized by droplet bridging. It occurs when a particle protrudes from an interface and simultaneously adsorbs onto a neighboring interface, stabilizing an intervening continuous-phase layer. However, the techniques to stabilize such emulsions remain rarely explored. We developed a simple and versatile strategy to engineer these bridged emulsions simply by tuning particle position at the interface (in situ) and adhesive forces [1]. Additionally, we examined the effects of particle surface charge, shape, size, and the influence of the addition of oppositely charged secondary particles of distinct wettabilities on the droplet bridging [1-2]. We thus determined the favorable conditions for designing bridged emulsions. The resulting bridged emulsions are mostly devoid of particles and provide a large accessible interfacial area, enabling their use as a microreactor for interfacial material engineering. Exploiting this feature, silica nanoparticles (NPs) are interfacially synthesized by hydrolyzing tetraethyl orthosilicate (TEOS in the oil phase) in the presence of an ammonia catalyst in the aqueous phase (Figure 1). A complete TEOS conversion is achieved within 2 days, compared to over 15 days at a flat interface. This significant reduction in the reaction time is due to the high oil phase volume to the surface area ratio of spherical droplets and the availability of a large total interfacial area for the reaction. This microreactor route facilitates control over yield and particle size by tailoring reaction time and TEOS concentration. Further, the potential of these microreactors in designing silica hollow microspheres and fluorescent nanoflakes is demonstrated by leveraging the interfacial synthesis at high TEOS concentration (Figure 1). This research establishes particle-bridged microreactors as a novel, high-yield, faster-conversion, and versatile pathway for interfacial NPs synthesis [3].

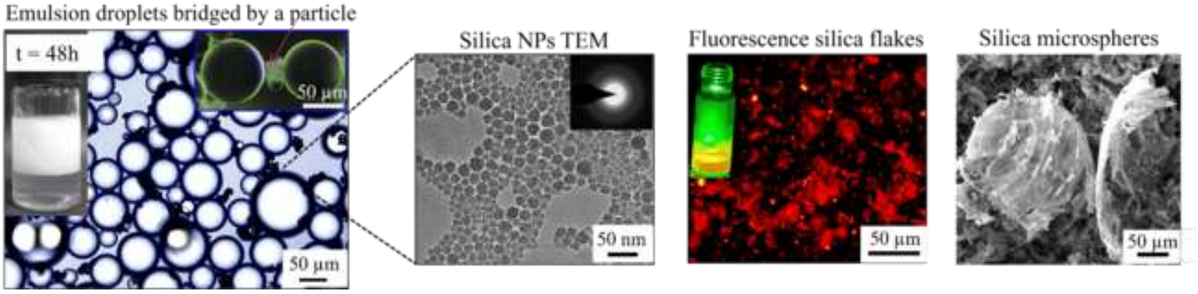

Figure 1: Bridged Emulsions as microreactors for interfacial material engineering

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Fatty Acids Incorporation As A Way To Reinforce Low Solids Network.

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Low solid formulations such as deosticks, lipsticks, lip balms often suffer from poor mechanical strength, leading to a significant risk of breakage during processing. In this study, we found that incorporating long-chain fatty acids greatly enhances the mechanical strength of these formulations. By controlling the fatty acid concentration, we were able to identify an optimal level that increases the system's modulus without negatively impacting its yielding behavior. Examination of the microstructure uncovers an interconnected network morphology responsible for the improved mechanical strength observed in the formulation.

Machine Learning Approaches To Classical Density Functional Theory: Towards Accurate Models Of Liquid Matter

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Classical density functional theory (cDFT) provides deep insight into the equilibrium structure of simple and complex fluids and can be extended to describe solid phases, all while remaining computationally efficient. However, the accuracy of this framework is fundamentally limited by the quality of the approximate free energy functional employed. Beyond perturbative expansions, no general and systematic approach currently exists for constructing accurate interaction functionals.

In recent years, several machine learning-based strategies have emerged to address this challenge. From this perspective, the problem can be formulated as an inverse task: determining an energy functional that reproduces the structural and thermodynamic properties obtained from simulations, all encoded in the *one-body* density. We review current data-driven machine learning approaches aimed at learning free energy functionals for classical systems [1].

In the second part, we demonstrate the effectiveness of these methods by applying them to realistic models, including molecular liquids [2, 3] and higher-dimensional systems [4]. A central bottleneck here is dimensionality: the high number of independent variables entering the one-body density distribution. Consequently, achieving full three-dimensional resolution in general inhomogeneous systems, while simultaneously treating particle anisotropy, presents a significant challenge. We show that physics-informed machine-learning networks enable this full 3D resolution [4]. Furthermore, for anisotropic particles (such as patchy particles), combining molecular density functional theory with machine learning offers a promising route toward a complete free-energy functional.

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Ultraslow Vorticity Modes in Colloidal Fluids

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Abstract: Flows at low Reynolds number are usually held up as the most orderly of fluid motions. Governed by the linear Stokes equations, they evolve deterministically, swiftly shedding any injected vorticity through microscopic viscous diffusion. This classical picture, however, rests on the assumption of a quiescent solvent. In colloidal and biological fluids, Brownian motion incessantly agitates the medium, provoking a natural question: can thermal fluctuations alone generate and sustain vorticity at microscopic scales in an otherwise overdamped environment? I will address this open question in this using high-speed confocal microscopy to resolve single-particle dynamics within a moderately dense colloidal suspension. We find that the vorticity associated with Brownian-induced hydrodynamic flows persists orders-of-magnitude longer than classical diffusion would suggest, decaying only with an ultraslow algebraic law over macroscopic timescales. Our theoretical framework attributes this remarkable persistence to hydrodynamic memory emerging from time-correlated, anti-persistent momentum impulses generated collectively by the Brownian particles. These findings show that vorticity−typically dismissed as transient in the Stokes regime−plays an active and enduring role in fluctuating low-Reynolds-number flows, with direct implications for transport, interactions, and collective behavior in complex fluids.

Desiccation crack prevention in clay-clay composite

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When water evaporates from interstices between particle aggregates, desiccation cracks occur [1]. Cracks in porous systems like clay, can alter its mechanical and hydraulic properties leading to damage of buildings as well as many other applications in geotechnical engineering. Recent advances in material have promoted the development of various novel composites, e.g. polymer-nanoclay composites, that have addressed the issue of desiccation cracks. These composites hold promise as advanced materials due to their superior properties, such as enhanced density, strength, high elastic modulus, and thermomechanical properties.

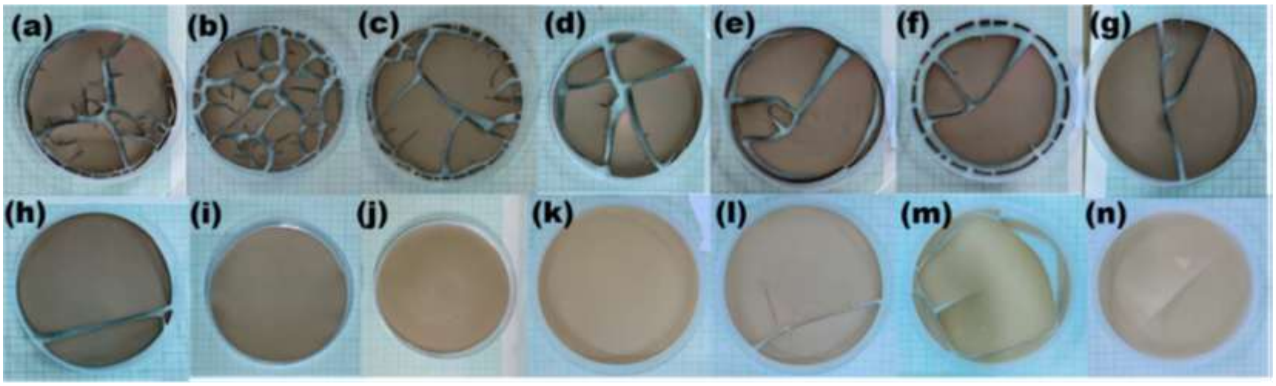

Fig.1. Crack pattern on dry films having of Laponite®:bentonite by weight ratio: (a) 1:19; (b) 1:9; (c) 1:5.66; (d)1:4; (e) 1:3; (f) 1:2.33; (g) 1:1.85; (h) 1:1.5; (i) 1:1.22; (j) 1:1; (k) 1:0.66; (l) 1:0.43; (m) 1:0.25; (n) 1:0.11.

Cracks due to desiccation of aqueous Laponite® films or aqueous bentonite films alone, are numerous and characteristic of the material. For the first time we report that when a aqueous composite these clays both belonging to the montmorillonite family is desiccated, the crack density is found to change according to the ratio of each clay present in the composite**.** *At a critical ratio of the two clays, cracks are totally suppressed, Fig (1).* The effect of varying film thickness, temperature and relative humidity on the critical ratio has also been examined. We have explained crack prevention based on SEM analysis of the composite where we show that the particle morphology is responsible for crack prevention at the critical ratio. The effect of temperature and relative humidity on the critical ratio have been explained in terms of energy optimization by the composite material [2].

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Fluorescently Mapped Biopolymer-Stabilized Water-in-Water Nanoemulsions for 5-Fluorouracil Encapsulation

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Abstract

Water-in-water (W/W) emulsions have emerged as a promising class of biocompatible soft materials for applications in pharmaceuticals, food systems, and advanced drug delivery, where stable nanoscale carriers are required to enhance solubility, bioavailability, and controlled release of therapeutics. However, the development of nano-sized W/W emulsions stabilized by non-toxic and biodegradable particles remains largely unexplored, particularly for drug delivery applications. In this work, we report a surfactant-free strategy for the fabrication of W/W nano-emulsions stabilized by chitosan nanoparticles (CS NPs) as biocompatible and cost-effective Pickering stabilizers for the encapsulation of 5-fluorouracil. CS NPs were prepared via ionic gelation using sodium tripolyphosphate (TPP) and systematically characterized in terms of particle size, zeta potential, and colloidal stability. Optimized nanoparticles with diameters of approximately 100 nm and positive surface potentials in the range of +16 to +40 mV efficiently stabilized dextran/polyethylene oxide (PEO) nano-emulsions generated by probe sonication, producing droplets with a mean size of ~800 nm. A key feature of this study is the use of fluorescein isothiocyanate (FITC)-labeled CS NPs, which enabled direct visualization of particle localization at the W/W interface. The appearance of a continuous green fluorescent layer confirmed interfacial adsorption of the nanoparticles and provided clear evidence of Pickering-type stabilization. Optical microscopy and FESEM further verified the formation of well-defined and stable droplets, with no observable coalescence for over 30 days. The nano-emulsions exhibited efficient encapsulation of 5-fluorouracil, achieving an encapsulation efficiency of approximately 76%, highlighting the suitability of this platform for the delivery of hydrophilic drugs. Overall, this study establishes chitosan-nanoparticle-stabilized W/W nano-emulsions as a robust and biocompatible carrier system for sensitive biomolecules and active pharmaceutical ingredients, with significant potential for biomedical and industrial applications.

Linking Microscopic Many-Body Interactions to Collective Behavior in Core-Shell Microgels through achine-Learned Potentials

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Core-shell microgels, consisting of a solid core covalently linked to a crosslinked polymer shell, are widely used as stimuli-responsive colloids,[1] yet a temperature-resolved microscopic understanding of their effective interactions–especially beyond the pair level–remains limited. In this talk we present a numerical framework to generate *realistic* core-shell microgels at different crosslinker concentrations and shell-to-core ratios, reproducing key structural features of experimental silica–pNIPAM systems across the Volume Phase Transition (VPT). After validating the single-particle architecture and its thermal response, we quantify interaction potentials between microgels as a function of temperature, extracting both two-body contributions and, crucially, the first *quantitative* characterization of three-body effects in a microgel system. While smaller than the pair term, three-body contributions are non-negligible and display a striking temperature dependence: they are predominantly attractive at low temperature, become repulsive at high temperature, and nearly cancel at the VPT, highlighting a subtle interplay between architecture, responsiveness, and many-body correlations.[2] Building on these microscopic insights, we then leverage a recent machine-learning (ML) approach to construct effective *many-body* coarse-grained potentials suitable for dense suspensions of colloidal particles.[3] By learning directly from fine-grained simulation data of swollen core-shell microgels in crowded conditions, the resulting coarse-grained models encode the emergent, environment-dependent character of microgel interactions and enable quantitative studies of collective behavior at high packing fractions, thus offering a route toward predictive, architecture-aware modeling of responsive soft materials under confinement and strong crowding.

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C-Oral-16

Morpho-Dynamics Of Liquid Cap In Desiccating Colloidal Droplets Over Partially Wetting Substrates

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The journey of a desiccating colloidal droplet begins with pinning of the contact line that involves enclosure of liquid cap region when probed with optical microscopy. This offers an alternative method [1] to characterise colloidal droplet desiccation rather than the conventional goniometry-based evaporation modes. Two regimes have been observed (pinned and retraction, Fig.1) over partially wetting substrates unlike the only retraction regime reported by Lilin et al. [1,2]. These can be correlated with the crack initiation in colloidal thin films. Further, the morpho-dynamics of liquid cap retraction of these desiccating colloidal droplets tracked as a function of particle content and particle length-scale (diameter) exhibits typical features.

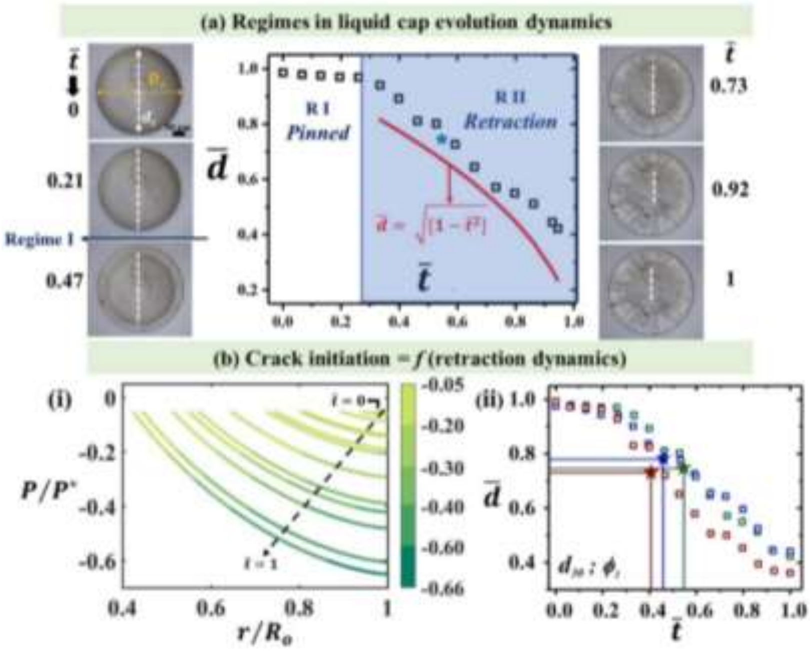

Figure 1 (a) Temporal evolution of the non-dimensionalised liquid cap diameter $\bar{d}$ ($\bar{d} = d_c/D_o$) of a desiccating colloidal droplet with dispersed particles of diameter, d_{30}, ϕ_1 demarcating the two regimes, Regime I or pinning stage and Regime II or liquid cap retraction stage, evolving with non-dimensionalized time, $\bar{t} = t/t_f$ where, t and t_f are the initial and final time instants of liquid cap formation. [liquid cap diameter, (d_c) (white, dashed line) and droplet base diameter (D_o) (yellow, solid line)] **Scale bar** : 50 μm. Timestamp of crack initiation is indicated with star symbol (★) in blue. Solid (red) line indicates fit of ($\bar{d} = \sqrt{1-(\bar{t})^2}$) as proposed by Lilin *et al.*[1] for universal evolution of liquid cap dynamics on relatively hydrophilic substrates **(b) (i)** corresponding pressure profile in particle deposit where arrow indicates the direction of progression of evaporation **(ii)** three distinct desiccating colloidal droplets (d_{30}, ϕ_1) representing three trials with crack initiation timestamp indicated by star symbol (★)

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Buckling in Spray-Drying Particle Laden Droplets: Experiments

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Fast evaporation of particle-laden drops produces particle-packed shells that buckle, giving rise to complex granule morphologies relevant to spray-drying processes. The transformation from an initially spherical shell to crumpled structures is driven by the compressive stresses generated by capillary forces acting on the shell. These morphological changes are governed by a universal dimensionless parameter that measures the competition between capillary stresses and the elastic strength of the particle packing. Experiments performed with single drops and spray-drying, where suspensions containing varying particle sizes, droplet sizes and moduli show remarkable agreement with this theoretical scaling over three orders of magnitude. The results demonstrate that the mechanics of shell formation and buckling are dictated primarily by particle size, mechanical properties, packing, and drying-rate-controlled shell evolution. This understanding provides a unified description of the transformations occurring in fast-drying, particle-laden droplets. A complementary observation from mixed particle–polymer systems shows that polymer distribution within the forming shell can alter deformation pathways. These results should enable design of hierarchically structured, buckle-free granules with varying porosity, surface composition and internal structure.

Engineering Anisotropic Colloids: Field-Directed and DNA-Encoded Pathways for Programmable Assembly

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Programmable bottom-up assembly of complex micro and nanostructures relies on two key requirements: (a) building blocks with diverse shapes and sizes, and (b) tunable interactions that can guide their assembly in a predetermined manner. Shape and surface anisotropic colloidal particles offer a versatile system to produce complex, reconfigurable structures. In this work we study programmable assembly of anisotropic colloids using two complementary systems: (i) TPM sphere-encapsulated magnetic hematite cubes, where the protruding cube creates an off-centered functional patch, and (ii) DNA-linked size-asymmetric magnetic dimers. In the TPM-cube hybrids, we achieve reconfigurable open lattices, stacks and clusters, controllable by electric field parameters. The displaced magnetic patch enables controlled formation of chains, flocks, and reversible oligomers using combined electric and magnetic fields. By striking a fine balance between the electric dipolar repulsion and the magnetic dipolar attraction, we demonstrate the versatility in the structural configurations, as well as their reconfigurability. In the second case, specially designed DNA strands are used to link two differently sized magnetic particles into dimers and short chains whose responses can then be controlled by applying external magnetic fields. Our results show that selective binding and field control in anisotropic colloidal systems can be utilized to produce adaptive architectures that can offer a pathway towards smart materials, switchable photonic crystals and design of microswimmers for targeted drug delivery.

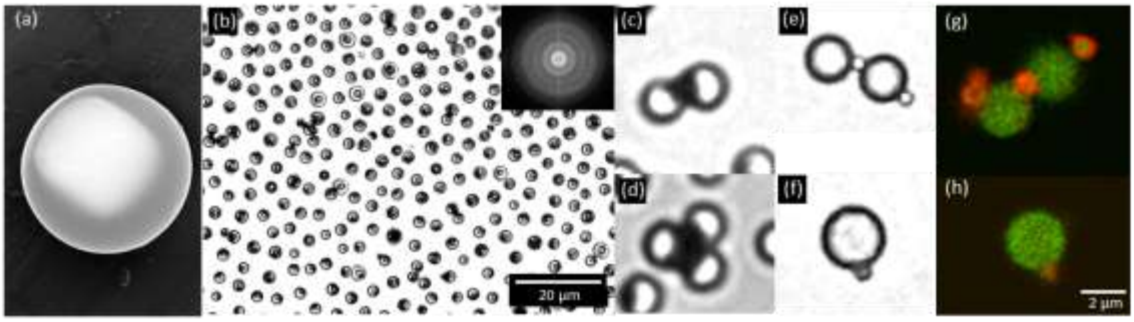

Figure 1: (a) SEM image of cube-TPM conjugate. (b-d) Structures formed by these conjugates in electric and magnetic fields. (e-h) Alternating chains and dimers formed by DNA mediated assembly (bright field and confocal microscopy images)

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Binary Big Atoms: Structure And Dynamics In Binary Mixture Of Dipolar Colloids

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Paramagnetic colloids have established themselves as "Big Atoms," enabling direct visualization of phase behavior, structural transitions, and interaction-driven organization at the single-particle scale. However, most studies have focused on monodisperse systems, where all particles share identical magnetic responses. In contrast, binary mixtures introduce competition in how two species align, assemble, and reorganize under external fields—offering rich behavior that remains largely unexplored. Here, we are interested the behavior of in 1D and 2D structures formed by a binary mixture of paramagnetic colloids that differ in size and magnetic susceptibility.

Under a static magnetic field, binary suspensions form one-dimensional chains that rapidly become kinetically frozen. This provides a unique opportunity to determine statistically preferred chain configurations and the positional roles of each species within a linear assembly.

When subjected to a rotating magnetic field, the same binary suspensions instead yield 2D clusters that continuously reconfigure. The field–magnetization lag, arising from species-dependent relaxation characteristics, drives rotational torques and neighbor-exchange events.

We want to explore binary Big Atoms as a minimal yet powerful model system for driven two-component materials, connecting colloidal self-organization with broader concepts such as driven segregation, pattern selection, and dynamics in heterogeneous populations.

Fluorescent Imaging And Micro-Rheology Measurements Of Structural Aging In Laponite Gels

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Structural aging in colloidal gels results from slow relaxation caused by restricted particle mobility and is accompanied by coarsening, the growth of a characteristic length scale [1]. How this structure develops under different strengths of attraction remains insufficiently understood. We address this issue in charged Laponite suspensions, where the interparticle attraction is controlled by adding salt [2]. Real-space fluorescent imaging demonstrates that the pathway of structural aging depends strongly on salt concentration. With weak attraction the samples remain macroscopically uniform, although coarse mesoscale domains gradually appear at long waiting times, as shown in the upper panels of Fig. 1a and Fig. 1b. With stronger attraction aggregation leads to heterogeneous structures that span coarse to fine regimes at the mesoscale together with macroscopic demixing, as seen in the lower panels of Fig. 1a and Fig. 1b.

Particle tracking provides complementary insight. Laponite-rich and -poor regions display distinct local rheology, and at low salt concentration the initially uniform suspension forms a homogeneous gel before heterogenization (Fig. 1b, 1c). In the colloid-rich region the displacement distribution Δx deviates from a Gaussian form, unlike in the colloid-poor region, reflecting submicron scale structural variation. We argue that the structural pathways revealed across salt concentrations can be interpreted as dynamically arrested phase separation governed by the strength of attractive interactions [3].

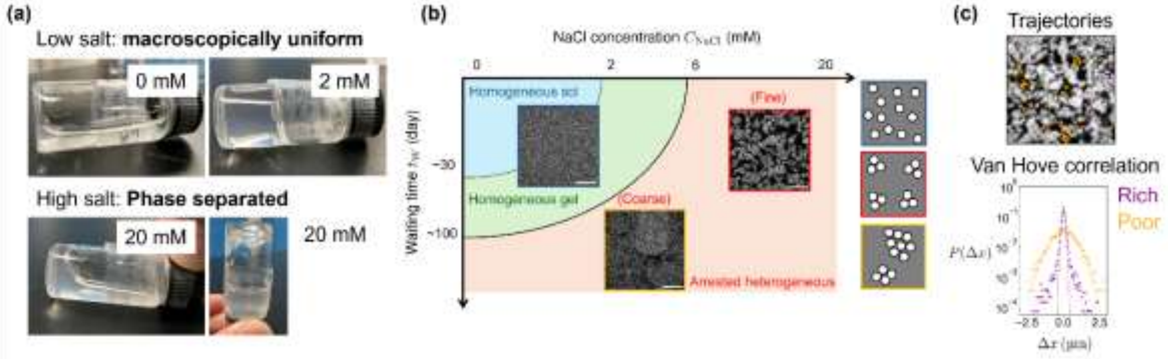

Figure 1: (a) Photos of 1 wt% Laponite suspensions at t_W = 307 days. (labels 0 mM, 2 mM, 20 mM denote NaCl concentration). (b) Schematic summary of aging behavior. Fluorescence images showing different aging structures: homogeneous, coarse, and fine aggregation. (c) Micro-rheology measurements by particle tracking.

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Beyond Linear Response In Colloidal Liquids

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Colloidal suspensions offer huge potential to provide new insights into the fundamental behavior of liquids, both because the particles' positions can be directly measured, and because their soft nature provides the unique possibility to go beyond linear response by exposing the system to strong fields. Here, we capitalize on this opportunity by directly measuring the response of a liquid to a strong spatially periodic external field in experiments, simulations and theoretical models. Strikingly, we observe a structural change in the direction perpendicular to the field variation, which evolves sensitively with the applied field period, as locally favored structures of the unperturbed liquid are selectively enhanced. These results open new research directions: by imposing artificial density modulations it is possible to extract structural information which are inaccessible to scattering experiments.

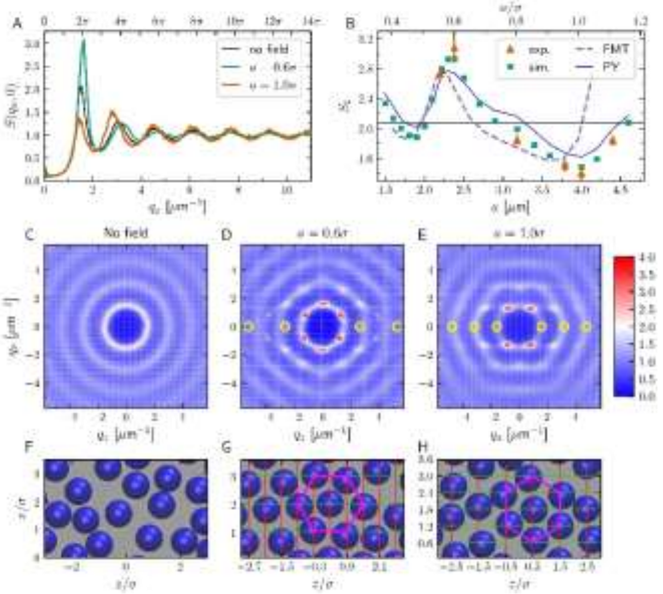

Figure 1: (A) Experimental structure factor in the direction perpendicular to the applied field. (B) Height of the first structure factor peak, (C) 2D structure factor of the field-free experiment. (D) and (E) 2D structure factor of the experiment with applied field. (F), (G) and (H) Illustration of stabilized locally favored structure for the field periods

C-Oral-22

Thermophoresis: The Role Of Non-Fickian Diffusion Current

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Thermophoresis is the phenomenon of transport of colloidal particles in a fluid in the presence of a temperature gradient. This phenomenon is similar to thermodiffusion observed by Ludwig [1] and Soret [2] in gas and other fluid mixtures. In either case, one observes the emergence of concentration inhomogeneities developing along the direction of the temperature gradient. Depending upon the excess concentration in the lower/higher temperature regions, the process is termed as thermophobic/thermophilic.

At the core of the non-equilibrium processes of thermophoresis are interactions at the solvation layer of the fluid-particle interfaces, which can depend on electrostatic forces, chemical forces, the structural dynamics of the colloid, hydrogen bonding, etc. Although such processes are extensively explored in experiments due to their wide range of applications, the theoretical understanding still lacks a general framework.

In this talk, we present a general theoretical framework that includes a non-Fickian diffusion current, proposed by Chapman in 1928 [3]. We show that the non-Fickian part of Chapman's diffusion current plays a major role in coupling the solvation forces, which are primarily believed to dictate the Soret coefficient as a function of temperature, to diffusion. We compare our observations with three experimental results based on aqueous solutions of Lysozyme, BLGA, and Poly-L-Lysine, and the match is quite good. For these test cases, we identify a general structure of the solvation force based on a simple equation of state. We also show that the local solvent density plays a major role in thermophoresis and thermodiffusion.

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Fluid Dynamics (FD)

Caustics and other things in particle-laden flows

Rama Govindarajan

ICTS-TIFR Bengaluru

I will describe an elegant way to look for caustics, or features supporting diverging particle concentration, in two-dimensional particle-laden flows. We will discuss what this reveals about caustics-forming particles. “Lucky” drops, which go on to become raindrops in a cloud, will be discussed in this context. We will then discuss some aspects of sand-dune reshaping and movement.

Generation of Nanoparticle-coated Functional Fibers Using Microfluidics and Their Application to Water Treatment

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Nanoparticle-functionalized fibers are widely used in areas such as catalysis, biosensing, tissue engineering, and the removal of pollutants from water. Conventional methods for producing these materials typically involve multiple processing steps, which frequently lead to non-uniform nanoparticle coverage and, as a result, diminished performance. In this work, we introduce a one-step fabrication strategy based on microfluidics to produce fibers with a homogeneous nanoparticle coating. Within a microfluidic platform, magnesium oxide (MgO) nanoparticles are deposited directly onto a jet of poly(vinylidene fluoride) (PVDF) solution as it undergoes fiber formation via solvent evaporation. The resulting fibers exhibit a consistent surface distribution of nanoparticles, which is essential for reliable functionality across applications. When applied to water treatment, these MgO-coated fibers act as an efficient adsorbent capable of simultaneously eliminating multiple heavy metal ions, including As(III), As(V), Pb(II), Cd(II), as well as mixed arsenic species [1]. Notably, MgO nanoparticles immobilized on fiber surfaces outperform free nanoparticles in contaminant removal, likely due to improved accessibility and effective surface area. This microfluidic fabrication approach can be readily extended to produce fibers coated with a wide range of nanomaterials, such as nanorods, quantum dots, and proteins, enabling broad applicability across diverse fields.

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Motion and flow of an electrically conducting particle subject to an oscillating magnetic field.

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An electrically conducting particle or drop experiences no force or torque in a steady magnetic field. Several interesting effects are observed when an electrically conducting non-magnetic particle experiences a time-varying magnetic field. When there is a rotating particle in a steady magnetic field due to applied shear, oscillating eddy currents are induced in the drop due to Faraday's law[1]. These impart a moment to the particle/drop due to Ampere's law. The cross product of the oscillating magnetic field and eddy current results in a steady component of the force density, which leads to a net torque on the particle when there is rotation. This leads to an antisymmetric part for the stress tensor, which is described by three antisymmetric viscosity coefficients. These result in a rheology modification which is qualitatively different from that for a symmetric stress tensor. When there is a spatially uniform oscillating field acting on an electrically conducting drop, the cross product of the oscillating eddy current and the oscillating magnetic field leads to a steady component of the Lorentz force density[2]. This generates internal circulation in the form of a dipolar flow field and a particle stress. When there is a gradient in the oscillating magnetic field, there is magnetophoretic moment of an electrically conducting particle. Expressions for all of these effects depend on the dimensionless parameter $\beta = (\mu_0 \kappa \omega R^2)^{1/2}$, which is the square root of the ratio of the oscillation period and the current relaxation rate in the conductor. Here, μ_0 is the magnetic permeability, κ is the conductivity, is the frequency ω and R is the particle/drop radius. The characteristic stress generated scales as $(\mu_0 H_0^2/R)$, where H0 is the magnetic field, and the characteristic velocity is $(\mu_0 H_0^2 R/\eta)$, where η is the fluid viscosity.

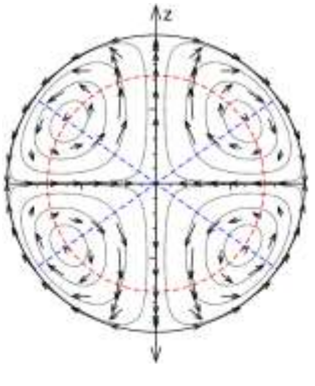

Figure 1: Circulation in an electrically conducting drop due to an oscillating magnetic field.

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[2] V. Kumaran, *J. Fluid Mech.*, 1014, A36, (2025).

Moving Contact Lines: Singularity, Flow Fields, Hysteresis, and Insights from Experiments and Simulations

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A moving contact line (MCL) forms when an interface between two immiscible fluids intersects a solid surface, a phenomenon encountered in everyday scenarios such as water drops sliding down a windowpane, spreading of paint on a dry wall, or ink-jet printing. What makes this problem fascinating is the singularity that arises at the moving contact line when the conventional no-slip boundary condition is applied to the moving solid. Most of our understanding of flows near a moving contact line are based on theoretical models in the low Reynolds number and low capillary number limit. A significant portion of experimental work on MCL has primarily focused on elucidating the angle-versus-speed relationship, with limited attention paid to the flow patterns. Recent results [2] from an experimental campaign involving a wide variety of fluid combinations, contact line speeds, and solid wettability shows that classical predictions from theory are consistent with experiments in spite of the singularity. Two main findings from the experiments include: (i) evidence of slip near the contact line, providing a direct pathway into how Nature resolves the singularity, (ii) anomalous flow fields for fluids with high hysteresis. The slip flow near the contact line is simultaneously accompanied by a rapid slowing down of the fluid along the interface. To understand the role of hysteresis, we resort to direct numerical simulations modelling dynamic variation of contact angle as a time-dependent contact angle boundary condition on the moving substrate. We show that shown that high frequency and low amplitudes contact line oscillations drives a steady streaming flow, directly competing with the primary flow. This competition can potentially alter the flow topology (Figure 1). A consolidated phase diagram is then generated to identify regimes to determine when existing classical theory [1] can safely be used, and when it fails.

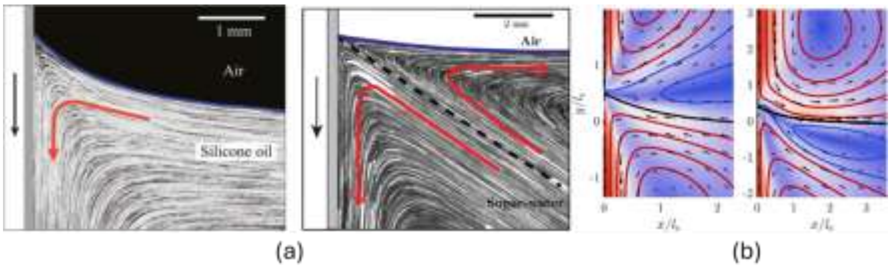

Figure 1: (a) Experiments showing rolling and split-streamline motion, (b) Simulations for low hysteresis with rolling motion (left panel) and high-hysteresis (right panel).

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Fluctuating Interfaces in Barotropic Beta-plane Turbulence

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Zonal jets manifest themselves as bands with sharp interfaces in the vorticity configuration. We develop an algorithm to track these fluctuating vorticity interfaces and systematically investigate their characteristic spatio-temporal behaviors. While the interfacial height fluctuations are typically sub-Gaussian, the corresponding *fluctuation speeds* exhibit wider, heavy-tailed distributions reflecting the influence of lateral dispersion induced by the zonal velocity profile along the interfacial contours. The temporal evolution of these fluctuations is further characterized through their power spectrum, displaying scale invariance in the frequency domain. The sharp, dense, shock-like features present in the time series of the *height* field suggest a possible lack of differentiability. We confirm this [1] by calculating the moments of the time-increments of the interfacial height fluctuations. Finally, the fractal nature of these boundaries is investigated systematically through a multifractal approach, revealing the non-trivial, complex statistics of interfaces in such geophysical, turbulent flows.

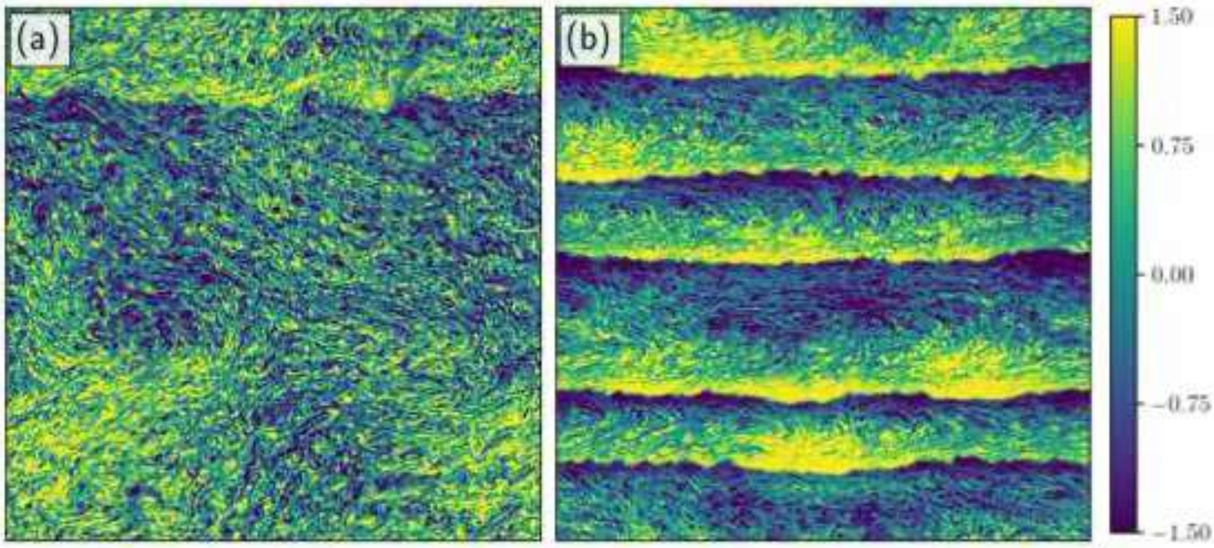

Fig. 1: Pseudocolor plots of the vorticity fields with (a) a smaller and (b) a larger zonostrophy parameter. Distinct jets, a key signature of zonal turbulence, are clearly seen which become more prominent for the case of larger zonostrophy prarameter.

[1] S. Sahoo and Samriddhi Sankar Ray, ArXiv: 2507.234

Cross-stream migration of spherical particles in shear and Poiseuille flows with viscosity gradients

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Spatial viscosity variation is often observed in biological and microfluidic environments, including regions near mucus layers, interfaces between fluids with different viscosities, and areas with temperature or solute concentration variations. While particle motion in quiescent fluid with viscosity gradients has been studied quite extensively, the particle migration is yet to be understood in confined channel flows with viscosity gradients. In this work, we fill this gap by theoretically and numerically investigating the motion of a force- and torque-free rigid spherical particle in confined channel flows with prescribed viscosity gradients. We consider both unbounded shear and pressure-driven (Poiseuille) flow fields, with viscosity varying perpendicular to the flow direction as $\eta = \eta_0\ (1+\epsilon Z)$, where η_0 is the reference viscosity and ϵ is gradient magnitude (refer figure 1(*a*)). To model the system, a multi direct-forcing immersed-boundary lattice-Boltzmann (IB–LBM) framework is used.

We find that, in presence of shear flow within a confined channel at finite inertia, the particle deviates from its constant-viscosity trajectory [1,2] and consistently migrates toward regions of lower viscosity (refer figure 1(*b*)). A similar viscophobic migration is also observed in Poiseuille flow (see figure 1(*c*)). Importantly, these migration dynamics are novel and arise solely due to the imposed viscosity gradient. The underlying hydrodynamic reason behind these viscotactic cross-stream migration is attributed to asymmetry in the local viscous traction distribution on the particle surface induced by the viscosity gradient, and its interaction with the background flow field. This behaviour may be interpreted as the cumulative effect of two competing mechanisms: (i) wall-induced lift forces and (ii) gradient-induced lift associated with the curvature of the external flow. We further develop an analytical theory in the Stokes regime, finding excellent agreement with the IB–LBM results. Overall, this study establishes that particles can undergo significant cross-stream migration purely due to viscosity gradients. Such passive and tunable control of particle trajectories offers new opportunities for microfluidic sorting and separation technologies.

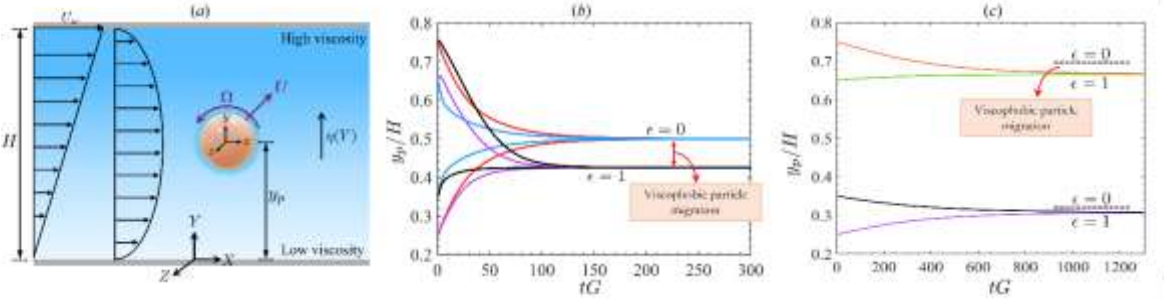

Figure: (a) Schematic of a translating and rotating sphere in a confined channel with viscosity gradient; Panel (b, c) depicts viscophobic particle migration in shear and Poiseuille flow, respectively.

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FD-Oral-06

Spectral analysis of the velocity relaxation in nanoscale channels

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Nanofluidics is an active research field with applications in everyday life, electronics, and medicine. In this talk, I will present a study of fluid velocity relaxation in nanoscale channels using molecular dynamics simulations and hydrodynamic modeling.
The relaxation dynamics are analyzed, using spatially resolved Fourier modes. Our simulations show that not only the mode with a wavevector equal to the external driving force is excited, but also smaller modes are excited. The relaxation can be found to be viscous at small wave vectors, transitioning to more viscoelastic behavior at larger wave vectors. Using Fourier mode analysis, we reconstruct the spatially averaged relaxation and identify that the dynamics are governed primarily by two modes: the system's largest wavelength mode and the external driving mode.
We conclude our talk by comparing the simulation data to two hydrodynamic models, the modified Maxwell model, taking into account non-local effects, and the Maxwell-Wiechert model [1].

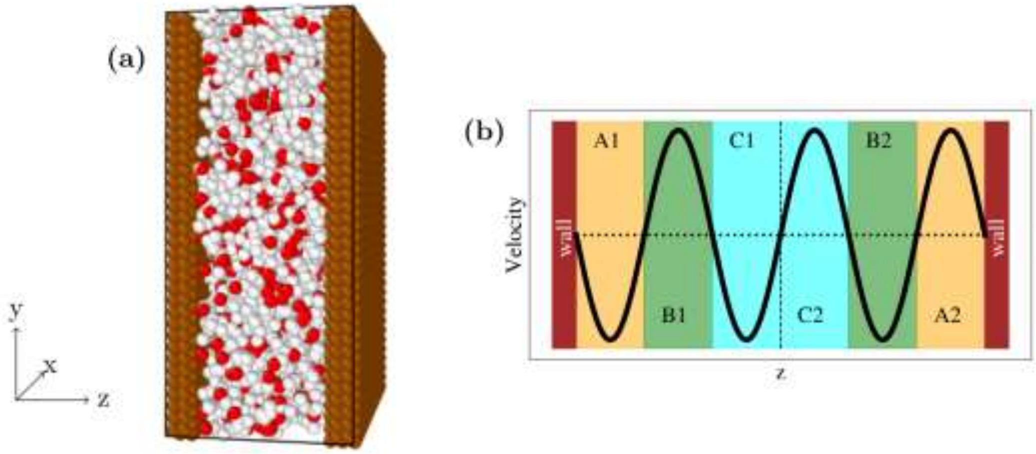

Figure 1: Schematic setup of the molecular dynamics simulation.

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Hydrodynamic singularities in soft matter system

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Soft-matter and free-surface flows often approach hydrodynamic singularities, where capillarity focuses inertia into slender Worthington jets and generates extreme stresses and droplets. In this talk, I compare two robust realizations—Worthington jets from drop impact on non-wetting (superhydrophobic) substrates and from cavity collapse after bubble bursting—and show how viscosity and polymer elasticity select the force signatures and droplet output. For impacting drops, experiments and direct numerical simulations (DNS) reveal two distinct peaks in the normal reaction force: an early inertial shock and a later peak that coincides with the onset of a Worthington jet at take-off [1]. By independently varying the Weber (inertia/capillary stress) and Ohnesorge (viscous/inertiocapillary timescales) numbers, we map the regimes of these peaks. A narrow window in this parameter yields an exceptionally intense, "singular" jet (fig. 1a). In contrast, for bursting bubbles in viscoelastic media, DNS identify droplet-ejecting jets, jets without droplet breakup, and complete jet suppression, controlled by the elastocapillary (elastic/capillary stress) and Deborah number (relaxation/inertiocapillary timescales) while leaving the capillary-wave speed essentially unchanged [2]. These results indicate concrete routes to tune, or inhibit, jet-mediated aerosol production relevant to printing and pathogen transport.

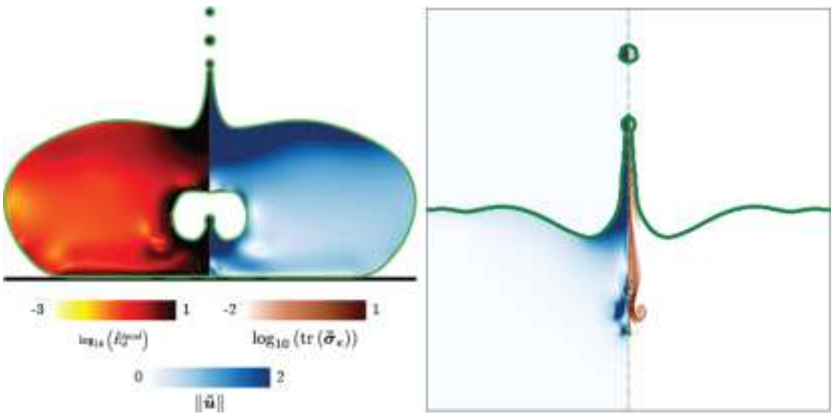

Figure 1: Representative numerical snapshots of Worthington-jet formation. Left: drop impact on a non-wetting substrate at the instant of the jet-associated force peak, showing viscous dissipation (left half, log scale) and velocity magnitude (right half). Right: bursting-bubble cavity collapse in a viscoelastic liquid, showing velocity magnitude (left half) and polymeric elastic stress (right half, log scale). The interface is outlined in green; green markers indicate ejected droplets.

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An Eulerian framework to compute the topological entropy of turbulent flows

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Deformation of material lines drives transport and dissipation in many industrial and natural flows. In this talk, I will report an exact Eulerian formula for the stretching rate of a material line, also known as the topological entropy, in stationary turbulent flows. The only requirement is a distribution of eigenvalues of the strain rate tensor and their decorrelation time. This can be easily obtained from a single wire probe at a fixed location, thereby eliminating the need for Lagrangian particle tracking which is formidable due to the chaotic nature of the flow. Numerical simulations reveal an excellent agreement between our theoretical estimate of the stretching rate of a fluid material line, over a wide range of Reynolds number. We believe that our results lend great utility in experiments targeting transport and mixing in many industrial and natural flows.

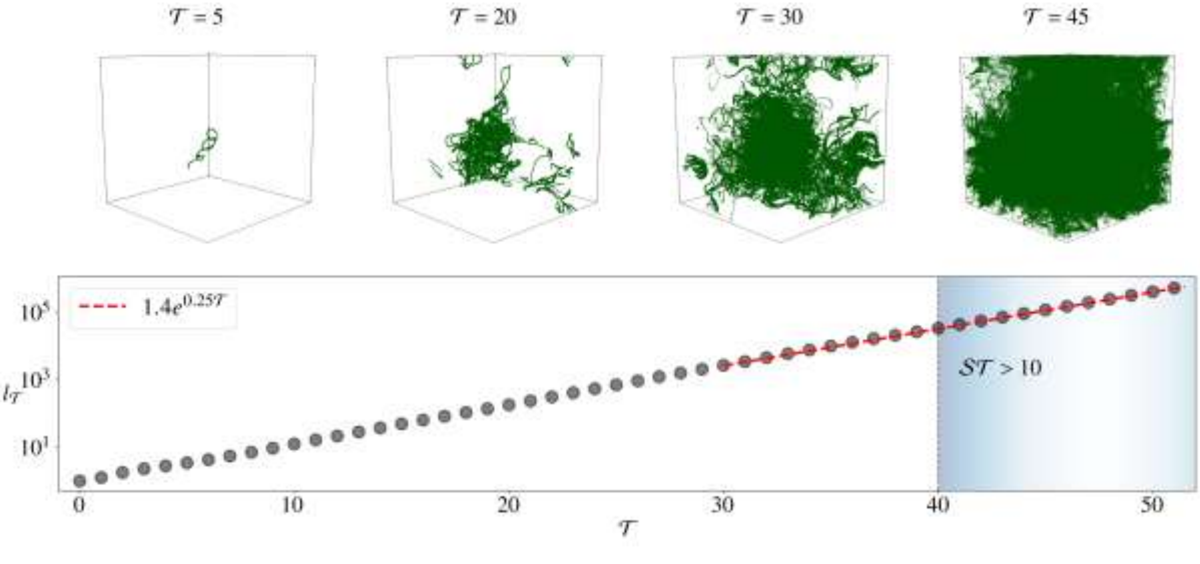

Figure 1: A typical time evolution of a material curve initialized as a straight line in a turbulent flow simulated at Re = 10^3. Our theory predicts this growth rate using just a spatial distribution of eigenvalues of the strain rate tensor.

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Interfaces, Surfaces and Membranes (ISM)

Leveraging Macromolecular Topology and Random Heterogeneity to Design Non-living Predators

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The fabrication of **biomimetic membranes for synthetic cells** that reproduce the key properties of living membranes remains a central challenge in soft matter. Liposomes offer biomimetic thickness, flexibility, and lateral mobility but lack robustness, whereas polymersomes are stable yet excessively thick and dynamically hindered due to entanglement of extended hydrophobic blocks. In this keynote lecture, I introduce a new class of biomimetic vesicles assembled from **ionically linked comb polymers (iCPs)** that resolves this long-standing trade-off.

iCPs are synthesized by appending anionic surfactants with lipid-long alkyl tails to cationic residues sparsely distributed along a hydrophilic polymer backbone. In water, iCPs self-assemble into vesicles, *i-combisomes*, with membranes consisting of a bilayer of hydrophobic tails flanked by tightly adsorbed polymer backbones. This architecture yields a cumulative hydrophobic domain length comparable to that of block copolymers, resulting in similar cohesive interactions and stability. However, breaking the hydrophobic block into multiple lipid-long segments suppresses chain entanglement, enabling biomimetic membrane thickness, ultralow bending rigidity, and lipid-like lateral mobility. A defining feature of this system is the **decoupling of membrane properties from polymer molecular weight**. In contrast to block copolymers, i-combisome assembly is governed by an *amphiphilic repeating unit*, allowing membrane thickness, flexibility, and dynamics to be independently programmed. By combining iCP libraries with simulations and quantitative biophysical characterization, we derived design rules for programming membrane properties and morphology.

At this point, I argue that prevailing mean-field descriptions of membranes miss a powerful design dimension. While topology and the packing parameter of the amphiphilic repeating unit are deliberately engineered, molecular heterogeneity inevitably emerges from the stochastic nature of polymer synthesis. This statistical distribution produces populations of iCPs in which most chains favor zero curvature for vesicle assembly, while a subset exhibits nonzero effective spontaneous curvature. We propose that units incommensurate with bilayer geometry store elastic frustration and selectively relax upon deformation, lowering kinetic barriers to invagination, fusion, and topological transitions.

This physics enables biological function. i-Combisomes readily fuse with synthetic and biological membranes and can engulf living bacteria. Exploiting this behavior, we engineered **phagocytic synthetic cells (PSCs)** that capture, engulf, and kill antibiotic-resistant bacteria through a purely physical, phagocytosis-like mechanism driven by the collective dynamics of topologically heterogeneous building blocks.

I conclude with a provocative perspective: these systems are not drugs but **adaptive, bioinspired materials**. By targeting the bacterial membrane, an evolutionarily conserved structure, through physical principles alone, phagocytic synthetic cells operate in a regime intrinsically robust against resistance, illustrating how topology, disorder, and frustration can be elevated from nuisances to functional design elements in soft matter.

Effective exponents for the diffusive coarsening of wet foams and analogous materials

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It is a long-standing puzzle as to why observed effective coarsening exponents cross over from 1/2 in the dry limit to 1/3 at the jamming transition, rather than in the very wet Lifshitz-Slyozov limit of dilute bubbles. I show this can can be explained in terms of approximate analytic calculation of the diffuse gas exchange rate between nearly kissing spherical bubbles. The result is a small logarithmic correction to a pure 1/3 power law, too small to be seen without data that is both more precise and over a larger growth range than is currently feasible to collect. Next, I show how the same approach can be generalized to jammed foams, where bubbles are modeled as truncated spheres with an average fraction f of their surface area consisting of soap films of thickness l separating them from neighbors. The result is an effective exponent that varies from 1/2 to 1/3 as f decreases from 1 in the dry limit to 0 at the jamming transition. With this theory, a key parameter that describes how microstructure changes with liquid content can be extracted from effective exponent data. This is demonstrated using prior data for two foams with different degrees of bubble-bubble cohesion.

Harnessing interfacial entropic effects in polymer grafted nanoparticle composites

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Nanocomposites based on polymeric materials have been extensively studied to understand and control the thermodynamics, flow, and mechanical properties of the underlying matrix as well to create new materials with diverse optical, electrical, magnetic, separation, catalytic, and biomedical properties. Using nanoparticles with grafted polymer chains usually overcomes a major hurdle in achieving enhancements in various properties by enabling better dispersion in the matrix while at the same time introducing a new parameter – interfacial entropy. This interfacial effect can be harnessed to control various properties of grafted nanoparticle composites, in particular their thermo-mechanical properties, viscosity, fragility, glass transition temperature (Tg), and dynamic heterogeneity.

In this talk we highlight, in particular, how this interfacial entropic effect can be harnessed to control various properties in thin films and membranes of grafted nanoparticle (GNP) composites. In particular, we highlight how interfacial entropy can be tuned to control evolution of phase separation in dynamically asymmetric binary polymer blends. By controlling the kinetics of GNP localization and interfacial jamming we demonstrate the ability to systematically arrest of phase separation. In addition, we also introduce an enthalpic parameter whereby we demonstrate control of phase separation evolution by tuning the extent of interfacial jamming of the GNPs.

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[3] Swain, A., Anthuparambil, N.D., Begam, N., Chandran, S. and Basu, J.K., 2025. Soft Matter, 21(18),.3443-3472.
[4] Ashish Biswas et al, Macromolecules (In Press, 2026).

ISM-Oral-01

A Unified Fabrication Strategy for Multifunctional Microstructures

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Natural surfaces offer powerful exemplars of how hierarchical structuring across multiple length scales generates tightly coupled optical and interfacial functions. The structural coloration of butterfly wings and peacock feathers arises from periodic micro- and nanoscale architectures that impose wavelength selective modulation of light through constructive interference, diffraction, and refractive index contrast. In parallel, the lotus leaf demonstrates how microstructures reduces the effective solid-liquid contact area and minimizes interfacial adhesion, thereby enabling efficient self-cleaning behaviour. Collectively, these natural systems illustrate how evolutionary optimization integrates hierarchical order to produce deterministic structure function relationships. Replicating such coupled photonic and wetting mechanisms in synthetic platforms is therefore central to the development of multifunctional bioinspired materials. [1] However, achieving these functionalities in optically transparent polymeric films at scale remains challenging. In this work, a simple fabrication strategy that integrates colloidal self-assembly with UV curable polymer replication via soft lithography is introduced. Surfactant assisted evaporative deposition of monodisperse polystyrene particles produces highly ordered colloidal template on glass substrates. The mirror structures of colloidal template is transferred onto PDMS mold and subsequently replicated onto UV curable polymers to yield transparent film with microstructures. The resulting UV curable film with microstructures exhibit angle-dependent structural coloration suitable for anti-counterfeiting applications, superhydrophobic behaviour reminiscent of the lotus effect, and reduced reflectance and glare compared to flat polymer film. This approach provides a low-cost, large area, and multifunctional route for producing bioinspired polymeric surfaces for optical, security, and advanced surface engineering applications as shown in Figure 1.

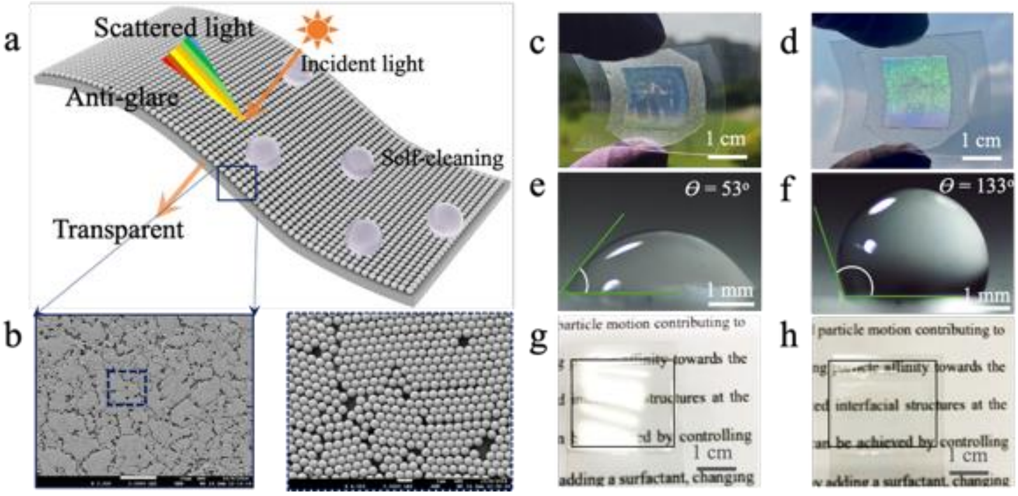

Figure 1. Multifunctional UV curable microstructures.

[1] A. Tiwari, S. Jae Lee, A.K. Thokchom*. Material Horizon, 12, 2689-2700.

Exotic Tribology of Soft Interfaces – Cartilages to Contact Lenses

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Tribology is the study of friction, lubrication, and wear of interacting surfaces in relative motion. While engine and machine-based topics dominate this field, the use of tribology in applications such as food and beverages, personal care, biological interfaces, etc., has gained massive traction in the past decade. These applications can be classified under the broader field of biotribology due to their interaction with the human body. The interfaces involved generally experience lower contact pressures than those found in conventional tribological systems. While this can be beneficial for testing, several key factors make the study of soft contacts especially challenging. One such factor is the selection and availability of proper surrogates for biological interfaces. Others include proper selection of test configurations in terms of the contact geometry, test parameters, conditioning of the specimen, and most of all, interpretation of the data obtained. The current work puts together case studies performed by the authors on select applications such as tribology of food and beverages, ocular system, skin/cosmetics/tissue, cartilage, implants, personal care products etc. The studies were carried out on an a rheometer-based tribometer with diverse contact configurations depending on the application. In addition to running extended Stribeck curves, tests were also carried out to determine the breakaway friction of the contact. The results presented here clearly demonstrate the importance of choice of specimen and its impact on the tribological characteristics of the interface. In certain cases, the right choice of specimen also amplified the differences in the behavior of the samples, see Figure 1. In addition to this, the tribological data from food and beverages were further analyzed through statistical means to generate a correlation between the frictional response and certain attributes of mouthfeel obtained by a sensory panel of experts.

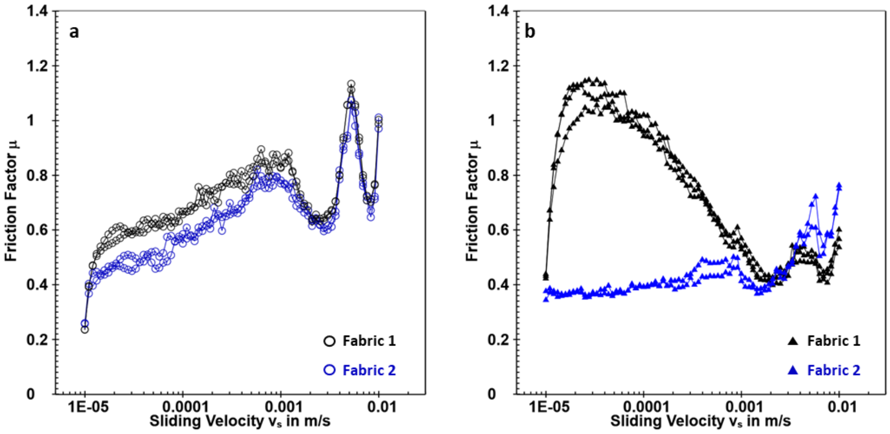

Figure 1: Graph depicting the frictional resistance of two different fabric materials against (a) polydimethylsiloxane pins and (b) artificial skin.

Probing cancer biomarkers using a biophysical approach

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We explored cancer cell-derived extracellular vesicles (EVs) and metaphase chromosomes to probe cancer biomarkers. EVs are naturally occurring lipid bilayer-enclosed nanoparticles involved in intercellular communication [1]. Hyaluronan (HA), a potential cancer biomarker, is a non-sulfated glycosaminoglycan. Our experiments revealed that Cancer EVs exhibited significantly increased HA surface densities compared to normal EVs [2]. We measured the contour lengths of single HA molecules on a cancer EV surface and assessed their mechanical properties [3]. We also elucidated the electrical properties of single-cancer HA-EVs [4]. These strategies could be realized as non-invasive cancer diagnostics in the future. Chromosomes are DNA-histone complexes essential for the inheritance of genetic information to the offspring, and any defect in them is linked to mitotic errors, cancer growth, and cellular aging. Chromosomal instability is a hallmark of different types of cancers. We addressed how an epigenetic modifier drug, valproic acid, impacts chromosomal elasticity and electron transport in cancer chromosomes. Using the physical properties of chromosomes, our multiparametric strategy offers a new scope for studying epigenetic dysregulations linked to cancer [5].

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ISM-Oral-04

Vortex-dipole interaction with a droplet

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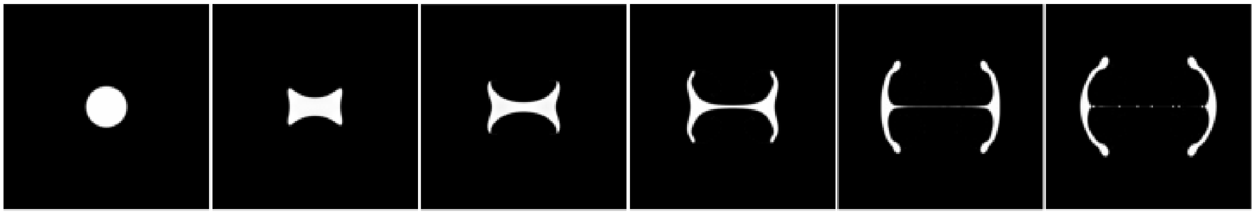
The interaction of a liquid droplet and vortex-dipole has a significant effect on the dynamics of the droplet [1]. In the present numerical investigations, it is observed that the droplet deformation is strongly dependent on the strength of the imposed vortex dipoles. The two-dimensional flow configuration is considered with two counter-rotating vortex dipoles, positioned symmetrically above and below a circular liquid droplet, which is located at the centre of the computational domain. This arrangement generates two converging jet-like flows which impinge on the droplet. The simulations are performed using an in-house developed lattice Boltzmann method solver based on a dual-distribution-function formulation for the simulation of multiphase flows [2]. The results demonstrate that, depending on the dipole strength, the droplet undergoes a range of deformation regimes, including periodic oscillations, neck formation, and eventual breakup. The study examines the effect of the density and viscosity ratio on the droplet dynamics. Figure 1 depicts the drop deformation from the initial configuration to the final breakup under the vortex dipole interaction. The density ratio between the drop and the surrounding is kept at 10.



t^*=0.0 t^*=0.001 t^*=0.002 t^*=0.004 t^*=0.008 t^*=0.01

Figure 1: Single droplet response under the vortex dipole interaction at different instances, the time is scaled with the capillary time scale, i.e., $t^* = t/t_c$, where t_c is $(\rho □^3/□)^{1/2}$

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Mycobacterial lipid remodels host cell lipid membranes to alter cytoskeleton dynamics fostering higher uptake

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Membrane-cytoskeleton interactions regulate processes such as exocytosis and migration, which are exploited by pathogens, are congruent with substantial modification of the membrane properties. Mycobacterium tuberculosis (Mtb)—causative agent of Tuberculosis—synthesizes chemically distinct glycolipids that are exposed on its outer membrane and interact with the membranes of host macrophages.[1-2] However, the effects of the structurally diverse *Mtb* glycolipids on the host cell membrane to fine-tune the host cellular response is unknown. In this work, we combined membrane biophysics, cell biology and microscopy to assess the effects of *Mtb* lipids on cell membrane mechanics, lipid diffusion, and cytoskeleton of THP-1 macrophages. [3-5] We found that Mtb lipids are transferred to macrophage membranes in a lab infection model, followed by modulation of macrophage membrane biophysical properties, and actin cytoskeleton. Extensive cellular FRET analysis revealed that the modulation of actin cytoskeleton is mediated by alteration in the localization and interactions between phosphatidylinositol 4,5-bisphosphate lipid, actin and actin regulatory proteins. This phenotype fosters higher bacterial uptake within the host and modulates cell migration by altering actin alignment and filopodia dynamics. Collectively, our findings highlight key molecular events and players involved in host membrane remodelling upon exposure to mycobacterial lipids during tubercular infection that enhances bacterial uptake within the host as potential therapeutic target.

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Space marbles: a soft matter-inspired concept for investigating the mechanical properties of lunar regolith

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In the current era of renewed interest in space exploration, the Moon is viewed as the stepping stone for achieving longer and sustained space missions aiming at both scientific exploration and space resources exploitation [1]. *In-Situ* Resource Utilisation is a powerful strategy for using locally available materials to build the infrastructure required for transforming the unwelcoming lunar surface into a critical outpost enabling deep space exploration. Lunar regolith, the unconsolidated material comprising rock fragments from the nano- to the macro-scale that covers the lunar surface, is a key resource in this context. To use regolith, however, the behaviour of this highly complex granular material must be well understood. Despite the significant knowledge acquired by both *in-situ* measurements and Earth-based studies of return samples, critical knowledge gaps regarding regolith physical properties, especially mechanical properties, remain. This is largely because only ~few grams of return samples are typically available for testing, whereas traditional methods often require ~hundreds of grams [2].

Driven by the need for metrology tools compatible with small-scale regolith samples, we propose using objects based on regolith-stabilised fluid interfaces, namely liquid marbles, gas marbles, and regolith films, to extract key mechanical properties of the constituent particles. A liquid marble is a drop coated by solid particles that are poorly wetted by the liquid [3]. A gas marble is a gas bubble enclosed by a liquid film containing partially wetted particles [4]. These millimetre to centimetre objects, which we collectively call space marbles, require regolith mass on the order of ~milligram or less. This critical advantage, combined with the recently highlighted link between liquid marble adhesion and friction between the particles and the substrate [5], opens the way for a metrology platform operating with minimal sample amount.

Here, we first discuss the formation, characterisation, and stability of space marbles prepared with regolith simulants, terrestrial particles that mimic the characteristics of lunar regolith. We then show how liquid marbles rolling on inclined substrates, and mechanical destabilisation of gas marbles, respectively reveal information about particle friction and interlocking. Beyond Earth-based studies with simulants, this metrology concept is intrinsically compatible with the constraints imposed by return samples, thus establishing a solid pathway towards future application to actual regolith. Beyond space resources science, the insights from this study may prove valuable for the characterisation of terrestrial granular materials that, much like regolith, feature particles with heterogeneous chemical and geometrical properties.

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ISM-Oral-07

Coarsening and interfacial morphologies in amphiphilic polymer-fluid blends

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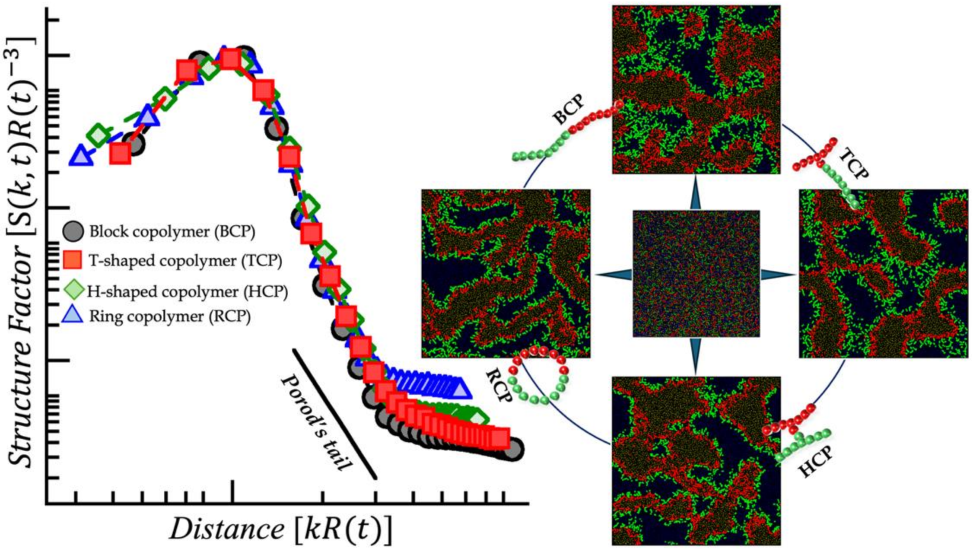
Polymer additives play a pivotal role in regulating phase separation kinetics and interfacial morphologies in multicomponent fluid mixtures.[1-5] By preferentially segregating to fluid–fluid interfaces, polymers act as effective modifiers of interfacial tension by controlling domain connectivity and hydrodynamic transport. Using the DPD simulation framework, we demonstrate how polymer concentration, chain length, stiffness, and topology govern the emergence of polymer-coated morphologies and alter coarsening pathways.[1-3] Polymer adsorption reduces the effective interfacial tension and enhances interfacial drag, leading to a systematic slowdown of domain growth and, under appropriate conditions, a crossover to arrested or saturated length scales. Architectural constraints further control interfacial packing and roughness, inducing deviations from classical scaling and Porod behavior.[3] These results establish polymer additives as versatile control parameters for tuning nonequilibrium morphologies and dynamics in phase-separating fluids, with direct implications for emulsion stabilization, rheological control, and the rational design of structured soft materials.[1-3]



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Hydration-induced structural evolution of intrinsically disordered proteins under confinement

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Intrinsically disordered proteins (IDPs) play a crucial role in soft and biological matter because of their structural flexibility, strong sensitivity to hydration, and tendency to undergo biomolecular phase separation. Despite their importance, a fundamental challenge remains in understanding how molecular disorder gives rise to organized structures at mesoscopic length scales, especially under spatial confinement. Addressing this question is essential for the rational design of responsive soft materials. Here, we use ultrathin films (10 -100 nm) of two representative IDPs as model systems: *silk fibroin*, which combines rigid crystalline segments with flexible amorphous regions, and *gliadin*, a highly disordered, glutamine rich protein. These systems provide an ideal platform to investigate how hydration drives structural evolution in confined protein films.

We design functional IDP thin films that exhibit stimuli-responsive conformational changes upon exposure to water vapor and other organic vapour. Small-angle X-ray scattering (SAXS), time-resolved synchrotron X-ray reflectivity, and spectroscopic ellipsometry are employed to probe conformational ensembles, interfacial structure, and swelling kinetics of these films in real time. By correlating hydration induced structural rearrangements with the intrinsic architecture of the proteins, this work seeks to establish general principles linking disorder, confinement, and emergent order. These insights provide a foundation for the development of programmable and adaptive biomaterials and will be discussed in detail.

Tuning lipid nanotube formation and interactions at biointerfaces through bilayer compositional control

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Lipid membrane asymmetry is commonly linked to differences between the two bilayer leaflets, but it can also exist within individual lipid molecules. [1] Although less explored, this intramolecular asymmetry plays an important role in determining molecular shape and driving self-assembly in aqueous environments.

In this work, we focus on the glycolipid ohmline (OHM), which exhibits a strong asymmetry between its hydrophobic chains. Below its main transition temperature, OHM spontaneously self-assembles into helical lipid nanotubes when deposited on Au surfaces. [2] These nanotubes are nanometers thick and can extend over several micrometers. In addition to its fundamental biophysical interest, OHM has also shown antimetastatic activity at low, non-toxic concentrations [3].

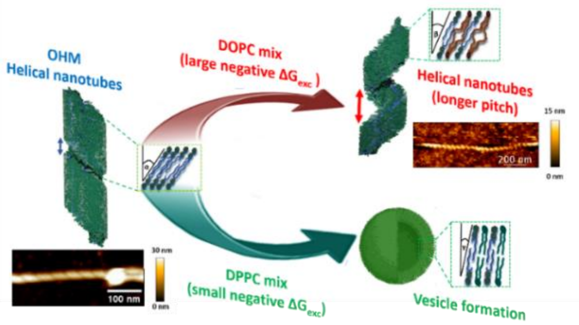

Fig. 1. OHM bilayers formed by glycolipid interdigitation can twist and bend into helical nanotubes. Incorporating selected phospholipids into OHM-rich bilayers modulates the self-assembly pathway, yielding a range of distinct nanostructures.

We then explore how mixing OHM with classical phospholipids affects nanotube formation and the balance between different self-assembled structures. By combining thermophysical measurements with atomic force microscopy, we relate bilayer composition to nanotube morphology. Our results show that simple changes in lipid composition allow precise tuning of both the formation temperature and structural features of the nanotubes (Fig. 1).

Finally, we demonstrate that this lipid-mixing strategy enables the fabrication of positively charged nanotubes, which in turn allows control over the kinetics and extent of cell adhesion. Yeast cell adhesion experiments highlight how surface charge, nanotube architecture, and membrane composition jointly regulate cell–lipid interactions. Overall, this work connects molecular-level membrane design to supramolecular structure and biological response, opening new perspectives for functional nano(bio)interfaces.

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Accelerating soft matter formulation: digital and computational approaches at BASF

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In today’s dynamic landscape, the rapid development of advanced formulations is crucial for innovation across soft matter industries, including home care, agriculture, and automotive sectors. Soft matter systems are at the heart of many modern consumer and industrial products. The ability to efficiently design and optimize such complex systems, while ensuring sustainability and performance, is a key challenge faced by both academia and industry.

At BASF, we leverage state-of-the-art digital and computational methods to accelerate the formulation process. Our methodology leverages high-performance computing resources, particularly the Quriosity supercomputer, in conjunction with close collaboration with experimental teams. By employing atomistic and coarse-grained models, we can simulate and screen hundreds of formulation candidates, reducing reliance on time-consuming laboratory iterations. This synergy allows us to probe microscopic interactions—such as those governing colloidal stability, interface formation, self-assembly, and rheological behavior, thereby offering deep mechanistic insights relevant to soft matter research.

We will present case studies demonstrating how our approach supports the development of sustainable, high-performance formulations. By integrating digital innovation with soft matter science, BASF is driving efficiency, reducing experiments, and enabling the next generation of materials for a more sustainable future. Our work underscores the crucial role of computational methods in advancing both fundamental and applied soft matter research.

Statistical physics perspective on mercury droplet spreading on thin metal films on glass

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Droplet spreading is a fascinating complex phenomenon, as the droplet spreads, reacts and dissolves on and into metal substrates. In high temperatures, one could have a large collection of liquid metals spreading on solid metals, with many applications in industry and material science. In room temperature, the only possible similar process is a mercury droplet spreading on a silver or gold thin film on glass. When this spreading is monitored top-view, rich and nontrivial spatio-temporal patterns of the advancing interface have been observed during the process.

In this talk we discuss the spreading of tiny mercury droplets (100-150 microns) on thin metal-on-glass substrate, with silver or gold thin films in various thicknesses (1000-4000 Å). The patterns in time and space of the advancing interface are analyzed using statistical physics and its relevant tools for the study of kinetic roughening, i.e. the *growth*, *roughness* and *persistence* exponents. Statistical physics exponents were calculated and sorted, thus providing insight into the complex spreading process and its dependence on the material, the film thickness, the internal morphology and the method of sample preparation.

The universality of the results has been examined by comparison with similar patterns of reactive wetting in *high* temperatures. More recent results for spreading on thin gold films suggest an even more complex picture of exotic instability patterns emerging towards the end of the process.

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How do membranes behave in microgravity?

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Pharmacology in space is the field concerned with how to dose drugs to humans in microgravity or on spaceships. On top of all the biological regulation mechanisms that act in the living being, there might be fundamental physical properties that change, in particular in microgravity. If so, these would need to be accounted for in the design of life-support systems and in the treatment of humans in such environment.

Soft-matter systems like giant unilamellar vesicles (GUVs) are ideal model systems to study any purely-physics effects of microgravity. Previous studies of small vesicles have already hinted at potential gravity-induced changes [1].

After a brief overview of the field of studying effects of microgravity on molecular biology, we report on measurements performed on GUVs during two sounding-rocket flights in the DLR MAPHEUS program to provide several minutes of microgravity conditions [2]. Molecular mobility was assessed using a specifically adapted UV-polarization measurement setup that is
robustly working under rocket-flight conditions. From the polarization we are able to deduce to rotational mobility of fluorescent molecules embedded in the membrane, and the changes in polarization intensity as the experiment changes from 1g to microgravity conditions, is a proxy to reveal gravity-induced changes in the dynamical properties of the membranes. We present these results as a puzzle to investigate possible mechanisms in how gravity might affect membranes, and provide an outlook for further microgravity experiments that (literally) shed more light on the issue.

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Prolonged underwater durability of liquid coated slippery surfaces

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Liquid or Oil coated slippery surfaces are typically vulnerable to shear forces due to external fluids flowing atop them. The surfaces which showed slippery properties in air media may become unstable when submerged underwater. Thereby, liquid films can be ruptured underwater as they are thermodynamically unstable and thus their functionality is not achieved. In this work, we will showcase that hydrothermally etched Aluminium 5083 alloy surfaces comprising of hierarchical micro and nano features have led to the formation of the thermodynamically stable oil films under 3.5 wt. % brine water. Aluminium 5083 alloys are intrinsically hydrophilic in nature and possess surface energy of 850±210 mJ·m^2 and its polar and dispersive components are 1.84±0.3 mJ·m^2 and 848±210 mJ·m^2, respectively. The spreading coefficient of silicone oil on Aluminium 5083 alloy surface in water medium is -13.941 mJ·m^2, indicating that the oil film is unstable underwater. Optical images also confirmed that the water droplets are stuck and oil is ruptured for untextured polished specimens just when submerged for <7 days. Nevertheless, hierarchically patterned surfaces possessing micro-pyramids, nano-flakes have shown stable oil film and slippery properties for up to 4 months of submersion time. This is very promising as the surfaces are not treated with any silanization or perfluorinated compounds. These surfaces have also showed excellent anti-corrosion properties and anti-biofouling properties. Such coatings are beneficial for marine, biomedical and sanitation applications.

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Membrane-mediated interaction of biomolecular condensates at biomembranes

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The spatio-temporal organization of biochemical reactions within cells is achieved through compartmentalization. Cellular compartments are either membrane-bound or biomolecular condensates, formed via the liquid–liquid phase separation of biopolymers. These condensates behave like liquid droplets with very low interfacial tension. They interact with lipid-bilayer membranes, where they can wet and deform their host membranes. Here, using the Helfrich Hamiltonian, triangulated membranes, and energy minimization, we investigate the wetting and wrapping of condensates at planar membranes. We find that condensates are wrapped when the condensate-cytosol interfacial tension is much higher than the condensate-membrane interfacial tension. The deep-wrapped state features a neck-stabilized droplet; the complete-wrapped state is suppressed. A very low condensate-membrane interfacial tension leads to complete wetting. We also calculate the membrane-mediated interaction between two partially wrapped condensates. Depending on the ratio of the droplet-cytosol interfacial tension and the membrane tension, the interaction potential is attractive or repulsive: high membrane tension induces repulsion by reducing the adhered area at short distances, whereas low membrane tension induces attraction via cooperative membrane deformation. Once two condensates come into contact, they merge into a nearly spherical droplet, reflecting the dominant role of interfacial tension in membrane bending. Our results show how the relative interfacial tensions and the membrane bending elasticity regulate wetting, wrapping, membrane-mediated interactions, and fusion, providing a quantitative framework for understanding condensate organization at biological membranes.

Microgel wrapping and encapsulation at membranes

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The softness of polymer gels plays a key role in their interaction with biological cells. Microgels with tunable size, shape, and deformability are a versatile system for understanding the interaction of elastic particles with lipid-bilayer membranes. [1, 2] Using a spring network model for the microgels and triangulated surfaces for the membranes, we study microgel-membrane systems using computer simulations and energy minimization. We determine the interplay of microgel and membrane deformations controlled by the competition between microgel elasticity and membrane bending rigidity. Our results predict an increased stability of partial-wrapped states for microgels with lower Young's moduli. [3] There is a discontinuous transition from oblate to nearly spherical microgels with increasing wrapping fractions. Understanding wrapping at lipid-bilayers can guide the design of the polymeric gels with optimal elastic properties for biomedical applications, such as targeted drug delivery vectors. We also encapsulate microgels with various Young's moduli within a spherical vesicle and shrink the gels at different rate. We observe a single bud for slow and a wrinkled membrane for high shrinking rates, similar to the osmotic compression of shells. [4] Vesicle-encapsulated microgels are promising drug delivery vectors because of their versatile surface functionalization possibilities. This study will allow us to comprehend blebbing of cells, which is common in the process of cell motility and death.

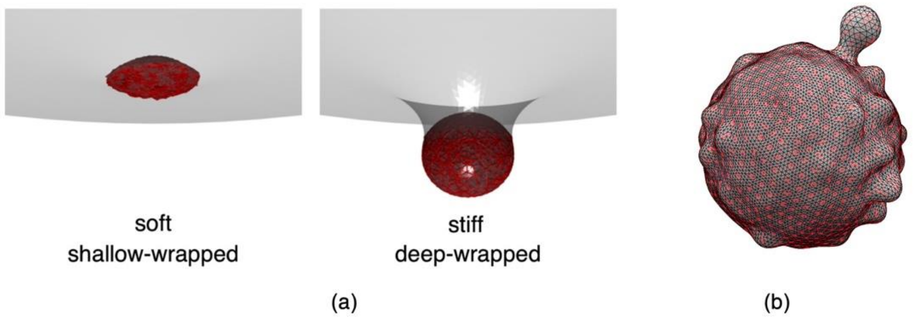

Figure 1: Microgels at lipid-bilayer membranes: (a) stable partial-wrapped states and (b) membrane bud formation for a vesicle-encapsulated microgel

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Investigation of interfacial behavior of extracted asphaltenes from bitumen precipitated in different non-polar solvents

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Bituminous asphaltene are most surface- active and structurally complex hydrocarbons that exert strong influence on interfacial phenomenon on water interfaces that effect their emulsion stability, wettability and flow characteristics in petroleum industry. Their precipitation and solubility characteristics are the key parameters to determine their interfacial behavior when dispersed in combination of various non-polar solvents and toluene. This work systematically investigates the interfacial behavior of extracted asphaltenes precipitated in various n-alkanes and their solubility in combination with toluene using comprehensive approach of interfacial rheology, fourier transform infrared spectroscopy (FTIR) and surface charge analysis by zeta potential measurement. Interfacial rheology revealed the evolution of interfacial film of all asphaltenes and maltenes obtained after precipitation in different non-polar solvents at the water interface and found high interfacial activity when same precipitated asphaltene was dispersed in combination with similar n-alkane and toluene or with lower carbon number n-alkane. FTIR analysis confirmed the presence of dominant surface-active groups and functionalities present which contribute to interfacial activity. Zeta potential was measured to determine the electrostatic stabilisation of all asphaltenes and maltenes. These combined results demonstrate a strong correlation between interfacial film strength, and dispersion stability and their dependence on solvent quality.

Phase separation bursting and symmetry breaking inside an evaporating droplet; formation of a flower-like pattern

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Pattern formation inside a liquid phase is a phenomenon involved in many different aspects of life on our planet. The droplet form of a liquid that evaporates can reveal patterns that depend on the chemistry of the droplet and the physical parameters involved. We observed a flower-like deposition pattern of micrometer-sized particles as a result of the evaporation of a droplet containing salt and a non-ionic polymer. We show experimentally that the phase separation of the polymer due to the salting-out effect causes a strong entropic flow, which manifests as vortices. The flow is called phase separation bursting flow, which leads to the axial symmetry breaking and the formation of a radially aligned flower-like pattern. We foresee that understanding the observed flow can provide insights into the fluid physics aspects of phase separation and may have implications for technical applications.

[1] *arXiv:2409.07095*

Mind the gap: Molecularly interfaced nanomaterials for next-generation sensing

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Nanostructures, such as nanoparticles and 2D materials offer a variety of fascinating properties, which render them promising for application in next-generation high-performance devices. In most device architectures, layers composed of an immense number of nanostructures act as functional components, rather than individual entities. As a result, material characteristics, such as charge transport or mechanical properties, not only depend on the individual nanostructures, but are strongly - if not predominantly - influenced by their interfaces.

Our work focuses on controlling and making use of such interfaces via introducing molecules to bridge the gap between nanostructures. Molecular cross-linkage results in tunable and functional hybrid materials, which exhibit properties such as pronounced tunneling-based strain sensitivity and chemiresistivity, that are highly desirable in sensing. In this contribution, we report approaches for cross-linking gold nanoparticles[1] and $Ti_3C_2T_x$ MXenes[2] with different molecular linkers. The influence of molecular interfaces and the ability to widely tune electronic, optical and mechanical properties of such systems via adjustment of their composition will be discussed. Eventually, applications exploiting the sensitive charge transport across functional molecular interfaces between nanostructures in sensing will be presented. These encompass tunneling-based strain sensors for healthcare applications,[1] highly sensitive microelectromechanical pressure sensors,[3] and chemiresistive sensors[2,4] for volatile organic compounds and water with high sensitivity and adjustable selectivity.

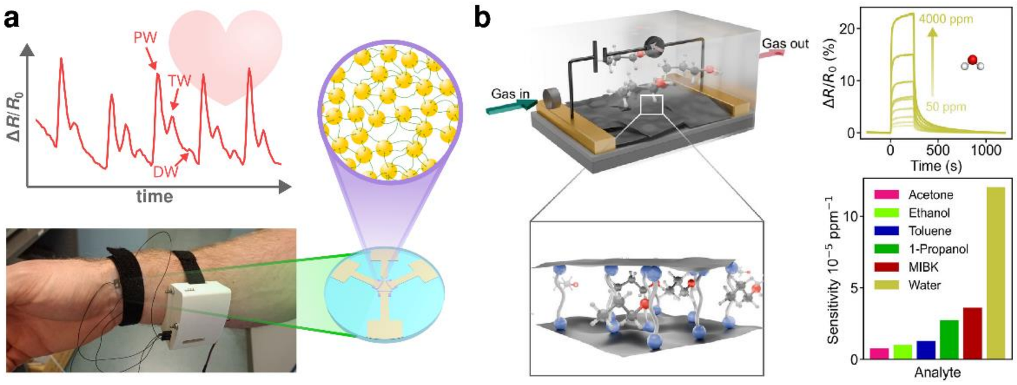

Figure 1: a) Wearable pulse and gesture sensor based on dithiol cross-linked gold nanoparticles. b) Diamine cross-linked MXenes for chemiresistive VOC sensing.

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Microstructure, dynamics, and liquid-to-solid transitions in lipid-stabilized interfaces probed by interfacial rheology

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Particles of lipids, such as monoglycerides, exhibit amphiphilic properties that allow them to easily adsorb to and stabilize both air-water and oil-water interfaces. As surface coverage increases, the interfacial particle network transitions from a fluid-like state to a solid-like state, with the specific characteristics of this state potentially being gel-like or glass-like, depending on the kinetics involved in the network formation.

In this study, we conduct a systematic investigation into the characteristics of liquid-to-solid transitions in lipid-laden interfaces through interfacial rheology. We perform frequency sweep measurements within the linear viscoelastic regime and analyze the results using a generalized Maxwell model, while carefully accounting for instrumental limitations and contributions from the subphase. We apply Winter's criterion [Winter, 2013] to extract the relaxation spectra, allowing us to deduce the nature of the liquid-to-solid transition in the interfacial particle networks at both air–water and oil–water interfaces, based on the scaling of the spectra with relaxation times. According to this criterion, gelation and glass-like arrest are viewed as inverse limiting cases, distinguished by negative and positive scaling exponents, respectively.

To probe yielding and nonlinear mechanical response, oscillatory shear experiments are conducted in the small-amplitude and medium-amplitude regimes. Distinct rheological signatures are observed for lipid networks formed at air–water versus oil–water interfaces. The nonlinear dynamic response is well captured by a modified Maxwell model commonly used in nonlinear rheology. Further insights into the microstructure at the interface are obtained as it undergoes yielding with increasing strain.

These findings enhance our understanding of lipid particle-stabilized interfacial networks and their differing mechanical behaviors at air-water and oil-water interfaces.

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Wettability gradient-driven capillary filling dynamics in tapered microchannels

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Capillary driven transport is ubiquitously found in nature, for example, the transport of water through plant xylem. It can also find potential application in autonomous flows in microfluidic networks. Through this work[1], we investigate the capillary filling dynamics in microchannels combining geometric tapering and spatially variable wettability. We employ high-resolution computational fluid dynamics (Navier–Stokes equations and the level-set method) to quantify the impact of stepwise, linear, and quadratic contact-angle profiles on the Laplace pressure, interface morphology, and flow velocity. For uniform channels and contact angles, the simulations reproduce the classical Lucas–Washburn regime, characterized by a viscous slowdown. In contrast, geometric tapering amplifies the capillary pressure gradient, sustaining or accelerating interface advancement. Tailored wettability gradients enable further control: decreasing the contact angle maintains flow, while increasing the angle toward 90° robustly halts motion, enabling on-demand interface arrest. These results reveal how geometric and interfacial patterning can be coupled for precision fluid manipulation, offering broadly applicable design principles for advanced passive microfluidic systems and programmable soft-matter transport.

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Interfacial phenomena in binary fluids: From surface adsorption to temperature-driven phase separation

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Close to phase transitions, the presence of surfaces and interfaces strongly influences the behaviour of fluids in and out of thermal equilibrium. In this work, we first investigate equilibrium interfacial phenomena by analyzing surface adsorption in a symmetric binary liquid confined to slit pores [1]. Based on molecular dynamics (MD) simulations, we have obtained order-parameter profiles near the bulk consolute point and for strong surface attraction. We characterize their critical scaling with temperature and confinement and compare these results against mean-field theoretical predictions. Complementarily, we study the phase separation dynamics far from equilibrium using a temperature-coupled Cahn–Hilliard–Cook framework [2]. We show that driving the binary fluid by a moving cooling source generates propagating thermal fronts and dynamically evolving interfaces between mixed and demixed regions. The observed morphologies and kinetics depend sensitively on two competing velocities associated with source motion and front propagation.

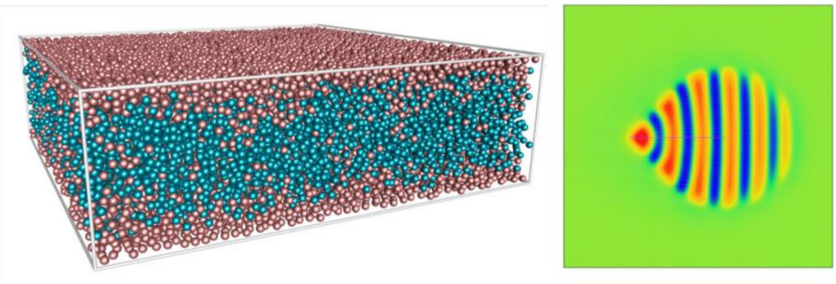

Figure 1: (a) surface adsorption of a symmetric binary liquid confined to a slit pore, studied within molecular dynamics simulations. (b) Interface formation far from equilibrium due to a heat source dragged through a phase-separating binary fluid.

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Structure of macromolecular liquids near an interface

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Structure of macromolecular liquids near a surface has been a subject of several investigations using different methods like mean-field theory [1] and Monte Carlo simulations [2]. The results from these investigations are useful in identifying the segment density distributions near an attractive or repulsive surface. The interaction between segments of the macromolecule and the surface in these studies are restricted to simple solvent mediated interactions depending on the concentration. In many applications specific interaction modifiers are combined with the macromolecular liquids for achieving modifications of the interfacial structure. The modifiers affect both the interaction between any two segments and the segments with the wall. Using field theory and Monte Carlo simulations we extend our understanding to look at the effect of addition of such modifiers to the evolution of the interfacial structure.

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Liquid Crystals and Anisotropic Matter (LC&AM)

Mesoporous Metamaterials and Aerogels from Liquid Crystals for Transparent Thermal Insulation

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Heating, ventilation, and air conditioning of buildings account for about 15% of the global energy consumption, but about 20% of this building-related energy is lost because of inefficient windows. Greenhouse emissions associated with producing and using this energy contribute substantially to climate change. Is there a solution to this challenging problem? Starting from the physical principles associated with energy loss through windows, I will describe our development of two different solutions in the form of visibly transparent, thermally super-insulating materials that may replace or retrofit the inefficient windowpanes of residential and commercial buildings. I will discuss how production of such unusual transparent mesoporous materials is enabled by mesoscale colloidal self-assembly and templating of orderly porous structures using lyotropic surfactant-based liquid crystals. With highly monodisperse pores controlled at the scale of nanometers, fabrication of such materials can be scaled to square-meter and larger dimensions by invoking self-assembly and simple processing. I will discuss how deployment of these porous aerogel materials can boost energy efficiency of windows, skylights and buildings in general [1-3], as well as allow for harnessing solar energy and then using it for both heating and cooling interior of buildings [3].

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Harnessing Topological Defects: Building, Moving, and Organising with Liquid Crystals

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Topological defects have long been central to various areas of physics, including cosmology, condensed matter, optics, and, more recently, active matter. Liquid crystals provide a uniquely accessible platform where such defects can be visualised, manipulated, and used to shape materials. When colloidal particles or droplets are dispersed in liquid crystals, the resulting elastic distortions act as multipolar sources, generating characteristic defect structures. These defect-decorated inclusions interact through anisotropic elastic forces, enabling programmable self-assembly and building of complex colloidal architectures.

Liquid-crystal emulsion droplets provide a complementary platform, where curvature and confinement stabilise characteristic defects, coupling topology to structure and function. By tuning anchoring and elasticity, defects can be used to guide organisation, template materials, and mediate interactions between droplets and particles. A further intriguing aspect arises when symmetry breaking in electrohydrodynamic flows leads to autonomous particle and droplet motion, turning these systems into active colloids. Understanding how defects control motility, transport, and collective dynamics presents rich experimental and theoretical challenges. In this talk, I will discuss our recent works on liquid-crystal colloids and emulsions, illustrating how topological defects can be harnessed for directed assembly and controlled transport in soft-matter systems.

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Boojums, Hedgehogs, Rings and Walls – Defects in Confined Nematics

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Nematics have orientational but not positional order, and often consist of elongated particles that align, on average, along a common axis or director. When confined within curved surfaces, the geometry and topology of the confining surface, together with the boundary conditions for the director field, all affect and often dictate how the material organizes. In this talk I will focus on the 3D confinement of nematics. In particular, I will discuss how we generate non-trivial confining spaces and how we quantify the order of the nematic inside them, paying special attention to the topological defects that we often observe. Inside tori with tangential anchoring, structures with broken reflection symmetry, as well as with pairs of boojums, are both observed. Applying magnetic fields results in the formation of inversion (Helfrich) walls both of the splay-bend and twist types. When confined inside surfaces with constant mean curvature, and subjected to perpendicular anchoring, we find states with either hedgehogs or rings. In many cases, the structures observed correspond to long-lived metastable states that are stabilized by the presence of large barriers between elastic free energy minima.

LCAM-Keynote-04

Micromechanics of Polydomain Nematic Elastomers

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Nematic liquid crystal elastomers (LCEs) are polymer networks containing rod-like mesogens that can order orientationally in response to temperature and mechanical loading. The coupling between network deformation and mesogen rotation provides nematic elastomers with enhanced viscoelastic dissipative behavior that enables superior acoustical damping, impact energy absorption, fracture toughness, and adhesion over a wide range of temperatures, frequencies, and strain rates. Nematic elastomers can be synthesized in a polydomain state containing locally aligned, micron-sized regions, or a monodomain state characterized by a single global director field. Polydomain nematic elastomers hold several advantages over monodomain nematic elastomers. They are easier to synthesize because they do not require an additional alignment step, and they exhibit an isotropic, rate-dependent soft-stress response, making them the more robust choice in many applications. However, the rate-dependent deformation mechanisms for polydomain nematic elastomers are poorly understood. The effects of domain size, orientation, and spatial distribution on the stress-strain and stress-relaxation responses remain unknown, which has hindered the development of physics-based viscoelastic models for polydomain LCEs.

To investigate microstructural deformation mechanisms, we have developed experiments using digital image correlation (DIC) to characterize the relaxation dynamics of the network and domains. We have also developed computational micromechanical models of representative volume elements (RVEs) of polydomain microstructures to investigate domain interactions during mechanical loading and relaxation. The thermomechanical behavior of the domains is described by a nonlinear viscoelastic microstretch model that captures rate-dependent mesogen ordering and director rotation, as well as network viscoelasticity. The macroscopic response of the polydomain material is then obtained through a homogenization formulation that integrates the contributions of differently oriented domains and accounts for their mechanical interaction. This multiscale approach predicts the macroscopic response of polydomain LCEs and the evolution of the director distribution and resulting texture under loading. Viscoelastic deformation and director reorientation emerge naturally from the homogenization, establishing a physically grounded link between domain-level physics and bulk material behavior at the representative volume element (RVE) scale.

The model reproduces key experimental observations of the polydomain to monodomain transition under mechanical loading and provides microstructural insight into the associated director reorientation. These results demonstrate the capability of the homogenization-based micromechanics framework to capture and interpret the complex nonlinear behavior of polydomain liquid crystal elastomers.

LCAM-Oral-01

Spontaneous Chiral Symmetry Breaking in Polydisperse Achiral Near-Rigid Nematogens

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Understanding chirality transfer from the molecular to the macroscopic scale poses a significant challenge in soft and biological condensed matter physics. Many nanorods of biological origin not only have chiral molecular features but also exhibit a spread in contour length leading to considerable size dispersity. On top of this, random backbone fluctuations are ubiquitous for non-rigid particles but their role in chirality transfer remains difficult to disentangle from that of their native chirality imparted by their effective shape or surface architecture [1]. We report spontaneous entropy-driven chiral symmetry breaking from molecular simulations of cholesteric liquid-crystals formed from achiral bead-spring rods with a continuous spread in contour length and marginal chain bending [2]. The symmetry-breaking is caused by long-lived chiral conformations of long rods undergoing chiral synchronization leading to a homochiral twisted nematic. A simple theory demonstrates that even without chiral synchronization, the presence of shape-persistent configurational fluctuations of non-chiral objects with inherent size-dispersity can be harnessed to bootstrap chiral synchronization.

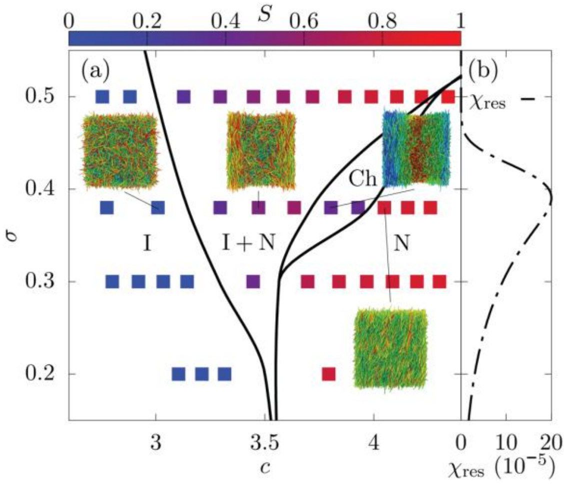

Figure 1: (a) Phase-diagram of soft repulsive near-rigid rods in the polydispersity-concentration (σ-c) plane. Points colored by global nematic order S. A spontaneously twisted cholesteric phase emerges at intermediate σ. (b) Residual chirality χ_res, predicted from a theoretical model, peaks at intermediate σ. Snapshots are colored by rod orientation.

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From Order to Chaos: Biomimetic Directron Dynamics in Nematic Liquid Crystals

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A hallmark of biological complexity is that systems often transition from directed, predictable behaviour to chaotic, irregular dynamics as parameters such as feedback strength, coupling, or environmental interactions change. The balance between order and chaos is essential in many biological contexts - order enables efficiency and reliability, while chaos provides adaptability, responsiveness and the ability to explore different energy states. Identifying new mechanisms by which such out-of-equilibrium systems can be artificially constructed is critical in the context of developing functional, intelligent, and adaptive soft matter.

In this work, we present biomimicking observations that showcase a fascinating transition from directed motion of directrons, in achiral nematic LCs, to a chaotic behaviour. The chaotic behaviour is characterized by the simultaneous presence of distinct directron families, each with its own trajectories. Each such class of directron can spontaneously transition to another, either randomly or through interactions with neighbouring directrons. with neighbouring directrons. Using simple energy arguments and a multi-body interaction model, we show that the distinct solitons each represent a unique energy state and that the transition behaviour is essentially driven by a competition between the stabilizing effect of LC surface anchoring and the destabilizing effect of the applied electric field.

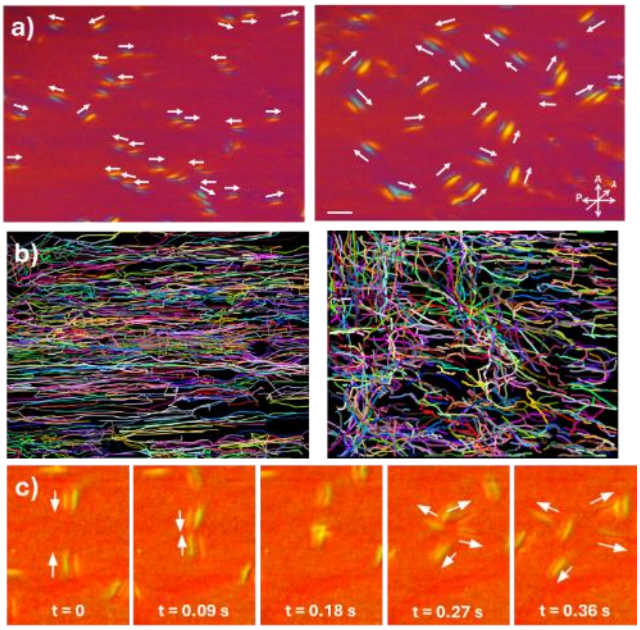

Figure 1 (a) Snapshots showing instantaneous directron trajectories at two different voltages. Directrons exhibit a directed (horizontal) to chaotic transition at high voltages. (b) Overall directron trajectories tracked over a period of 5 sec. (c) Timed snapshots showing directron collisions leading to splitting of directrons. Directrons adopt random trajectories post splitting – building chaos in the system.

The unique combination of distinct directron families and directron splitting further enables the mimicking of several features of a living system, such as the "run-and tumble" motion of individual bacteria, formation of higher order motile structures such as pairs and chains of directrons, mediated by directron-directron interactions. Additionally, our work also demonstrates that high-energy directrons can spontaneously split into two low-energy daughter directrons thus mimicking spontaneous biological "fission" process. Collectively, these observations demonstrate that LC directrons can mimic the rich behaviours observed in active living systems, thus opening new realms in the field of bio-inspired soft matter for applications such as accelerated transport, colloidal cargo delivery and focused energy transduction.

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Generation and control of nanosecond light by light in liquid crystal

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The unique combination of softness, anisotropic properties, strong responsiveness to external fields, and surface alignment capabilities makes liquid crystals exceptional materials for a wide range of photonic applications, including flat-panel displays, light modulators, tunable Filters, entangled photon sources, and lasers. Despite these advantages, integrating liquid crystals at the microscale into photonic devices that match the performance of silicon-based chips while consuming less energy, operating solely with light, exhibiting biocompatibility, and enabling self-assembly has largely remained unexplored. In this work, we present a soft-matter photonic chip that integrates tunable liquid-crystal microlasers with laser-microprinted polymer waveguides. We demonstrate dynamic control of liquid-crystal microlaser emission using nanosecond optical pulses and introduce a resonant stimulated-emission depletion mechanism for all-optical switching. This approach paves the way for a new generation of photonic integrated devices that are not only biodegradable and biocompatible but also suitable for applications in medicine, wearable photonics, and optical logic. We believe soft-matter photonic circuits will surpass traditional solid-state photonics by significantly reducing fabrication steps, eliminating toxic materials, improving energy efficiency, and ultimately creating a new paradigm in soft-matter photonics. [1]

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Quasi-universal thermodynamic behavior of convex-hard-body fluids

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The macroscopic properties of a system are influenced not only by thermodynamic variables such as temperature, volume, and particle number, but also by the characteristics of its constituents. This is especially true for anisotropic bodies, prompting the question of whether particles with similar geometric features exhibit similar thermodynamic behavior. We address this question by performing two-dimensional Monte Carlo simulations of various polygons with number of edges k and deformations of a disk (i.e., $k = \infty$). We discover that, for fixed k, the compressibility factor $Z_k(\eta)$ as a function of the packing fraction η collapse into a quasi-universal narrow band, provided the polygon's areas are identical and their shapes are moderate deformations of their regular counterpart. The resulting quasi-universality classes exhibit hierarchical structure $Z_k(\eta) > Z_{k+1}(\eta)$ (η) for η which becomes more and more pronounced with decreasing deformation. This associates the thermodynamic behavior of convex bodies with geometrical universality classes characterized by the number of edges. Our findings provide a geometric framework for predicting fluid behavior across the full density range of the isotropic phase. The emergence of distinct bands tied to particle geometry challenges the notion of a single universal equation of state and opens a new avenue for understanding shape-dependent thermodynamics.

Knots as Particles: Machine-Learned Potentials for Interacting Topological Solitons in Liquid Crystals

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Knotted field configurations exhibit nontrivial topology and particle-like behavior [1], yet their practical use in condensed matter has been limited by the difficulty of stabilizing them. Recently, stable knotted solitonic textures—heliknotons—have been realized in chiral liquid crystals, that self-organize into adaptive crystal assemblies through elastic-distortion-mediated interactions [2]. However, modeling their interactions remains challenging due to their highly deformable field configurations and strong anisotropies.

Here, we develop machine-learned effective interaction potentials that model heliknotons as quasiparticles described solely by their geometric centers and orientations. The coarse-grained potentials trained on fine-grained simulations using the Frank-Oseen free-energy functional accurately capture the strongly anisotropic and chiral interactions and reproduce experimental heliknoton assemblies. Our results demonstrate that heliknotons can indeed be quantitatively described within a particle-based framework, opening the door to computationally efficient modeling of other topological textures across diverse condensed matter systems [3].

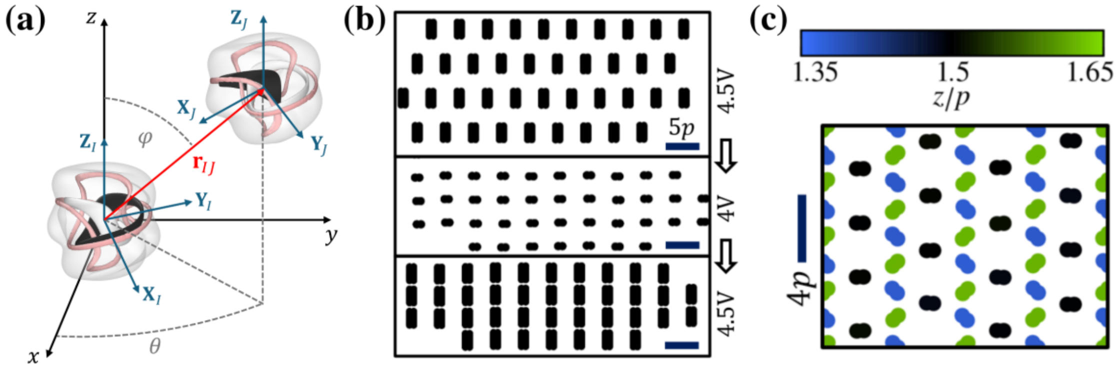

Figure 1 (a) Coarse-grained representation of a pair of heliknotons using their geometric centers and orientations. (b,c) Simulations using the coarse-grained potential showing self-assembly of heliknotons into various 2D and quasi-3D crystals.

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Polymers and Gels (PG)

PG-Keynote-01

The role of thermal annealing on the viscoelastic properties of model polyisoprene vitrimers

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Vitrimers have emerged and an important class of dynamic covalent networks that undergo associative, reversible bond exchange, and exhibit properties between thermosets and thermoplastics. In an effort to understand these properties, we investigated model polyisoprene-based vitrimers synthesized via condensation reaction of α,ω-aldehyde-functionalized polyisoprene and tris(2-aminoethyl)amine), by anionic polymerization and high-vacuum techniques. We investigated a range of molar masses from 2 to 54 kg mol^{-1}, corresponding to a broad range of crosslink densities. Our findings indicate that thermal annealing over unusually long time drives these metastable networks toward a pseudo-equilibrium state through imine exchange and cluster rearrangement. In particular, it leads to pronounced increase in both storage and loss moduli, accompanied by a shift of the SAXS peak to lower scattering wave vectors. These trends indicate that enhancement of elasticity is linked to the reorganization and growth of clusters, as further confirmed by scanning electron microscopy measurements. Networks with higher crosslink density exhibit the strongest effects with the largest value of storage modulus. At the other end of the spectrum, networks with high molar mass display two plateau regions, reflecting contributions from entanglements and crosslinking groups (clusters). Overall, these results combining structural and rheological probes clearly demonstrate that thermal annealing is crucially important in assessing and tailoring the structural and mechanical properties of vitrimers, something that had not been appreciated before.

Work in collaboration with Arcangela Russo, Benoit Loppinet (Crete), Saibal Bhaumik, Konstantinos Ntetsikas, Nikos Patelis, Nikos Hadjichristidis (KAUST), Einat Nativ-Roth, Moshe Gottlieb (Ben Gurion University), Benoit Loppinet, Evelyne Van Ruymbeke (Louvain), and supported by the EU (Rebond network).

PG-Keynote-02

Charged Macromolecules: Assembly, Dynamics, and Transport

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Charged macromolecules, dispersed in aqueous media, are ubiquitous and are manifest in all forms and functions of all Life. Inevitably, charged macromolecules exhibit a variety of enigmatic puzzles that are unprecedented in uncharged polymers. Examples include (1) even similarly charged polymers clump together under conditions of extreme electrostatic repulsion, (2) diffusion of gigantic charged macromolecules can be as high as that of a small metallic ion exhibiting the “ordinary-extraordinary” transition, (3) apparent violation of Einstein’s law of diffusion in crowded aqueous media at room temperature even if we were to wait for very long times comparable to the age of the universe, and (4) polymers made of neutral-polar monomers can move under an electric field, but only in one direction and never in the opposite direction. We identify the nucleus of these enigmatic phenomena as the confluence of concurrent occurrence of three long-ranged correlations arising from the chain connectivity, electrostatics, and hydrodynamics. We will highlight the fundamental principles behind charged macromolecules in unraveling the above puzzles. Implications of these principles are abundant in Life processes and technological innovations.

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Crowders as Architects: How Size and Attraction Reshape Polymer Collapse and Aggregation

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Macromolecular crowding is commonly interpreted in terms of excluded-volume and depletion effects, yet many crowded environments also involve attractive interactions between polymers and crowders. In this talk, I present a systematic simulation study of how such attractions modify polymer conformations and aggregation behavior. Using coarse-grained molecular dynamics, we examine neutral and charged polymers over a range of polymer–crowder interaction strengths, crowder sizes, and densities. We identify two distinct collapse mechanisms: a bridging-driven collapse induced by small attractive crowders that penetrate the polymer coil, and a confinement-assisted collapse induced by larger crowders that exclude polymers into interstitial regions. These mechanisms lead to structurally distinct collapsed states and, near transition thresholds, to non-monotonic and reentrant conformational behavior. We further show that the collapsed state induced by crowder-mediated bridging is similar to that obtained from strong intrapolymer attraction or electrostatic correlations, suggesting a common underlying physical mechanism. The results provide a unified framework for understanding how crowder size and attraction control polymer collapse and aggregation in crowded soft-matter systems.

PG-Keynote-04

Biological gels of the plant world-Mechanics of plant mucilage and physiological relevance

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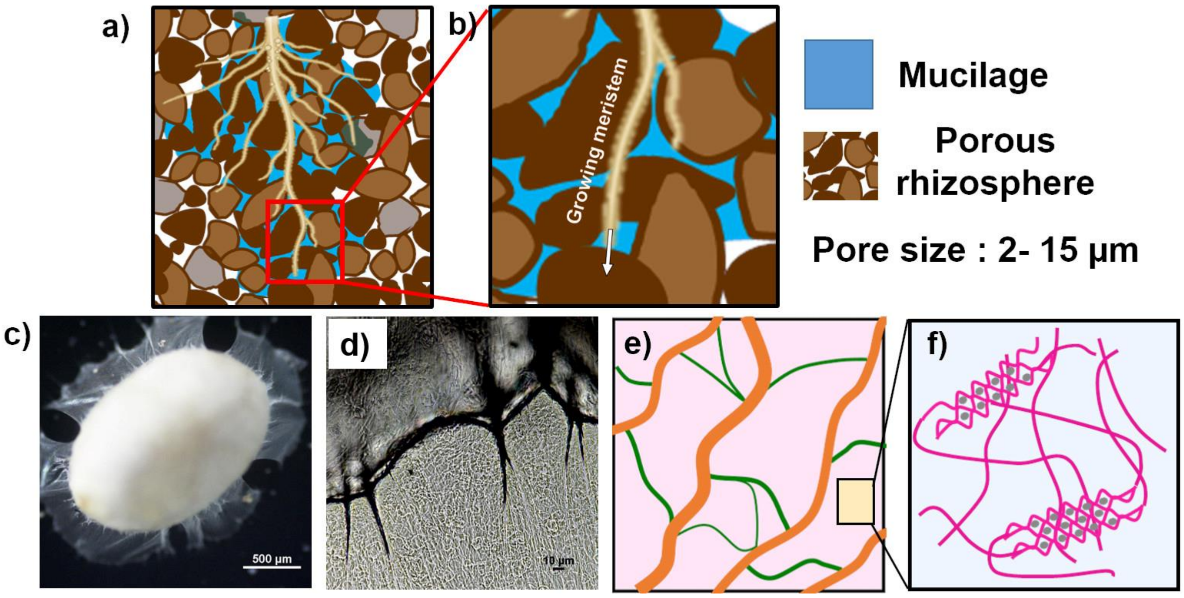
Plants produce viscoelastic high-molecular-weight gel-like materials known asmucilage to serve different physiological and ecological functions. Mucilage is a polysaccharide-rich substance, but also contains proteins, minerals, and lipids. Depending on the plant species, mucilage secreted by the roots, seeds, leaves, and stems can vary in composition, structure and functions. Mucilages are functional gels which helps in water retention, structural integrity, nutrient uptake and protection. They also assist in root penetration through the soil by lubrication, helps in seed germination, act as barrier against drought and stress and as medium for plant-microbial interactions in the soil. These ionically crosslinked gel networks differ microstructurally in different species and in different parts of the plant. We use various rheological and structural analysis techniques such as, large amplitude oscillatory shear (LAOS), microrheology using optical traps and tribo-rheology to study polysaccharide gels produces by plants of different species. Rheological studies on controlled compositions of pectin based gels to understand the nature/role of ionic crosslinking is carried out in parallel. The results are used to understand the structural contributions of these hydrogels to the physiological/adaptive functions in plants. Adaptations to grow in different climate, soil and environmental conditions are shown to correlate strongly with the structure and rheological behaviour of these polysaccharide gels.



Evolution of Linear Viscoelasticity across the Sol-Gel Transition

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Gels comprise synthetic polymers to colloidal systems and represent a unique state of soft matter characterized by a space spanning percolated network swollen by liquid solvent. As a material transforms from a flowing sol state to a soft solid-like gel state comprising of a space-spanning percolated network, its mechanical response undergoes a remarkable change. At the critical gel state, which is an intriguing unique point between the sol and gel states, the relaxation of stress becomes scale-free, and characteristic relaxation times diverge. In this work, we investigate how the linear viscoelastic properties, especially the storage and loss moduli, evolve as a system passes through the critical gel state while undergoing sol-gel transition. By examining the evolution of relaxation spectra with respect to the degree of crosslinking, we identify the conditions under which the relaxation spectrum evolves in a symmetric manner on both sides of the critical gel point, a puzzling behavior reported for many colloidal and polymeric systems. Furthermore, we show that the proposed framework offers a unified perspective on the emergence of critical scaling and hyper-scaling exponents during the sol–gel transitions and how two parameters, the critical relaxation exponent and the dynamic approach exponent, dictate the entire evolution of the linear viscoelasticity around the critical gel point.

Complex Coacervates in Complex Environments

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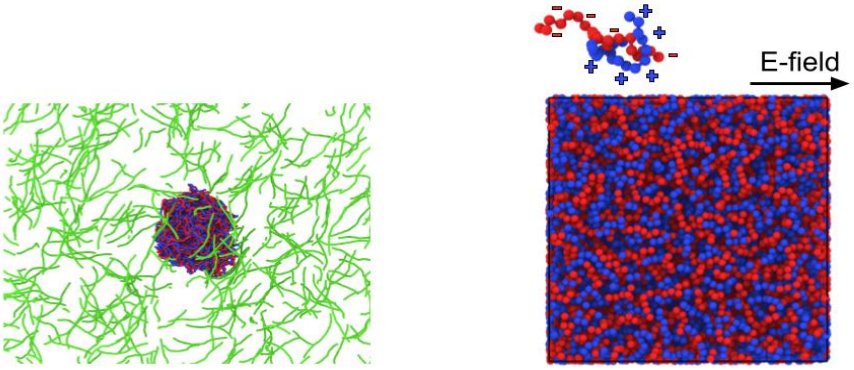
Complex coacervation is the phase separation of oppositely charged polyelectrolytes, resulting in a polymer-dense coacervate phase and a polymer-depleted supernatant phase. Coacervation is crucial for many biological processes and novel synthetic materials, where the environment is often complex. Yet, a complete understanding of complex coacervates is still lacking, mainly due to the large parameter space involved in coacervation and the out-of-equilibrium conditions often encountered in experiments. In this talk, I will discuss multiple molecular dynamics simulations of complex coacervates, including how the salt resistance of coacervates changes depending on the presence of neutral molecules (crowders) in the local environment, and how applying an external electric field to coacervates shows many of the characteristics of applying shear to neutral polymers.



Complex coacervate in a crowded environment

Complex coacervate under E-field

Figure 1: Simulation snapshots of complex coacervates in a crowded environment and under an external electric field.

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Computational design of stimuli-responsive biopolymer-grafted nanoparticles for therapeutics

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Polymer grafted nanoparticles are hybrid materials where the organic or inorganic nanoparticles are functionalized with polymers of desired chemistry [1,2]. These (bio)polymers can be biomolecules such as DNA, proteins or can be stimuli-reponsive synthetic polymers. These hybrid materials find attractive applications in biodiagnostics and therapeutics. In my group, we have worked on designing these grafted nanoparticles in an aqueous environment such as that found inside a crowded living cell to mimic the solution milieu that these nanoparticles encounter in biological fluid once administered into the patients [3-5]. Using molecular dynamics simulations, we have designed ss-DNA functionalized gold nanoparticles in molecular crowded environment of mixed amino acid solutions. Examining the solvation thermodynamics indicates that the solvation free energy of these nanoparticles is dependent on the effective size of the nanoparticles, which in turn is determined by the chemistry of the molecular crowders [6]. The ss-DNA sequence dependent change in the effective size of the nanoparticles is observed. We have also designed generic polymer- capped nanoparticles that are responsive to the change in temperature. By tuning the hydrophobicity of these polymers, a similar response to the size of the nanoparticles is observed as found by varying the temperature. Furthermore, thermo-sensitive gold nanoparticles have also been designed that are capped with PNIPAM (Poly-N,N'-isopropylacrylamide) chains. The competition between polymer collapse transition and polymer-nanoparticle interactions determines the overall effective size of the nanoparticle in presence of temperature stimulus. The microscopic view of the effects of molecular crowding, hydration and biopolymer chain chemistry on the structure, stability and stimuli-response of grafted nanoparticles, will be discussed.

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PG-Oral-04

Effect of Dipeptide Terminal-End Associations on the Structural, Dynamic, and Rheological Properties of cis-1,4-Polyisoprene in Natural Rubber

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The terminal structures of cis-1,4-polyisoprene (PI) chains are critical in governing the exceptional mechanical performance of Hevea natural rubber (NR). PI chains exhibit distinct terminal groups, classified into ω and α types. Experimental studies have identified two types of ω terminal ends and six α terminal ends ($\alpha 1, \cdots, \alpha 6$). In this study, we investigate five polyisoprene melt systems, each with unique combinations of terminal groups: hydrogen (H), ω, ω', $\alpha 5$, and $\alpha 6$. The ω represents a dimethyl-allyl group connected to two trans-isoprene units, while the ω' group consists of an alanine dipeptide (ADP) segment linked to a dimethyl-allyl and two trans-isoprene units. The $\alpha 5$, and $\alpha 6$ groups correspond to the ester- and hydroxy-terminal groups. The studied systems include hydrogen-terminated $_{\mathrm{H}}\mathrm{PI}_{\mathrm{H}}$ (PI_0), ester-terminated $_{\omega}\mathrm{PI}_{\alpha 5}$ (PI_{V}), hydroxy-terminated $_{\omega}\mathrm{PI}_{\alpha 6}$ ($\mathrm{PI}_{\mathrm{VI}}$) and dipeptide-terminated $_{\omega'}\mathrm{PI}_{\alpha 5}$ ($\mathrm{PI}_{\mathrm{V'}}$) and $_{\omega'}\mathrm{PI}_{\alpha 6}$ ($\mathrm{PI}_{\mathrm{VI'}}$). Using all-atom molecular dynamics simulations, we analyzed static (end-to-end distance , radius of gyration, Kuhn length) and dynamic (end-to-end vector autocorrelation, Rouse modes) properties. Intermolecular interactions were examined via radial distribution functions, potentials of mean force. Strong hydrogen bonding between ω'- ω', and ω'-αgroups leads to slower dynamics and the formation of stable clusters in $_{\omega'}\mathrm{PI}_{\alpha 5}$ and $_{\omega'}\mathrm{PI}_{\alpha 6}$ systems. These clusters act as physical junction points (PJPs) stabilized by β-sheet-like hydrogen-bond networks between dipeptide terminal ends. The stress-stress autocorrelation function, $G(t)$, reveals a chain length-dependent slowdown in relaxation dynamics for ($\mathrm{PI}_{0,\mathrm{V}}$) systems, with slower relaxation observed at $N = 96$ (N is the number of monomer present in each chain) compared to $N = 24$. In contrast, ($\mathrm{PI}_{\mathrm{V'}}$, $\mathrm{PI}_{\mathrm{VI'}}$) chains exhibit faster relaxation at $N = 96$, attributed to weakened end-group associations and the absence of large clusters that dominate the $N = 24$ systems. These findings demonstrate that β-sheet-like PJPs may be key to the outstanding properties of NR.

Universal center-of-mass scaling shapes segment fluctuations and chromatin dynamics

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We show that cancellation of internal forces together with spatially uncorrelated noise generically enforces a universal $1/s$ scaling of the center-of-mass (COM) diffusivity for polymer segments of contour length s, independent of model details. Within an active generalized Rouse-Langevin (A-GRLE) framework for fractal polymers in a viscoelastic bath with weak activity, we derive closed-form links between segment COM motion and the short-time behavior of two-point fluctuations. The same COM law predicts transient $\sim s^{-3}$ tangent-tangent correlations along the contour following a temperature quench. Reanalyzing recent two-locus chromatin tracking, we extract a dynamic COM exponent ξ=0.77±0.16, suggesting topological constraints. These results identify model-independent signatures of collective polymer dynamics and clarify that the observed Rouse-like scaling of chromatin loci reflects transient, unentangled dynamics with an inevitable crossover to an entangled regime at longer times.

PG-Oral-06

Shear-Wave Emission from Interacting Cavitation Bubbles in Gelatin

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Shear waves in soft elastic media provide valuable insight into local mechanical properties and dynamic processes such as cavitation, fracture, and tissue deformation. We investigate shear wave generation in gelatin gel induced by the collapse of two neighboring cavitation bubbles using high-speed imaging and polarization-based shear wave tracking. A mechanical model approximating the bubbles as time-dependent lateral point-forces reproduces the main features of the observed propagating waves.

Shear waves in soft tissues have emerged as a powerful tool in biomedical research, enabling quantitative assessment of viscoelastic properties [1], diagnostic elastography, guidance of minimally invasive procedures, and fundamental studies of stress transfer in biological materials [2]. Previous works have demonstrated that single bubble collapses can launch shear waves when symmetry is broken by boundaries or neighboring structures [3,4]. Building on these earlier works, we examine here the shear waves emitted by two closely spaced cavitation bubbles.

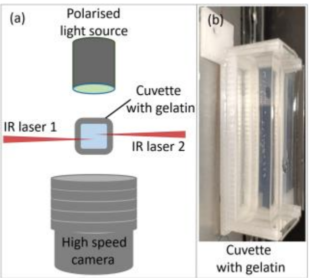

Fig. 1 (a) Experimental setup (b) Customized cuvette with gelatin gel

We employed two infra-red laser systems (Litron Lasers Ltd, Nano S and T) (Fig. 1(a)) to nucleate two adjacent cavitation bubbles within a 4 wt% gelatin gel housed in a customized cuvette (Fig. 1(b)). Polarized illumination and a high-speed camera (Photron Inc., Crysta) records the resulting birefringence patterns induced by stresses within the gel.
High speed images (Fig. 2 (a)) show that the bubbles expand to maximum sizes (first frame), collapse, re-expand, move towards each other, and gradually move away (in consecutive frames). The corresponding retardation images (Fig. 2(b)) reveal that the shear waves form at first collapse, they propagate radially and form complex patterns as shown in subsequent images.

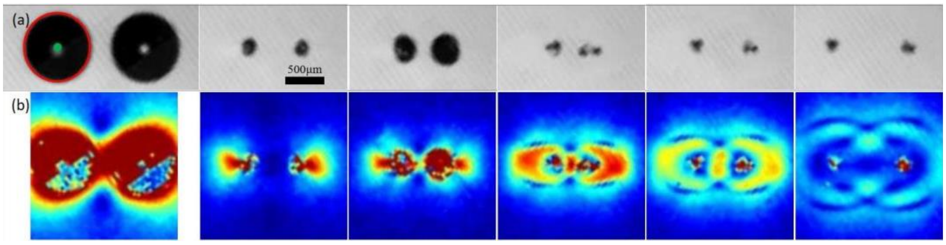

Fig. 2 (a) Image of two bubble collapsing from its maximum size, rebounce, collapse towards and then move away. (b) The corresponding retardation images showing the generation and propagation of shear waves. Time in microseconds for the frames are 47, 93, 107, 187, 253,

To interpret these observations, we modeled the system as two point sources subjected to time-dependent lateral forces. The force is derived from the lateral displacement of bubble 1 (red outline, bubble center is green (Fig. 2(a))) and the wave propagation speed is taken from experiment to be 0.9 m/s. The calculated shear displacement field reproduced the experimentally observed wavefront geometry, validating the hypothesis that the lateral jetting motion acts as the dominant shear source. This work demonstrates that multiple bubble interactions can be harnessed to generate controlled shear waves in tissue-mimicking media.

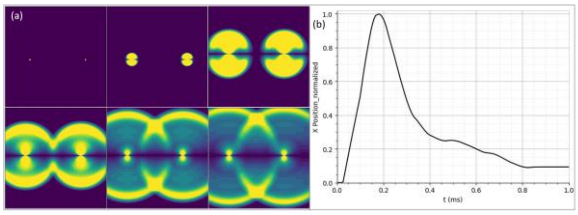

Fig. 3 (a) Calculation of propagation of shear waves from the movement of two point sources in a linear elastic medium. (b) Normalized movement of bubble 1(red circle, Fig. 2(a)) in time.

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Universal speed limit for supersonic crack propagation in viscoelastic solids: An exact analytical solution

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Classical linear elastic fracture mechanics predicts that tensile (mode I) cracks cannot exceed the Rayleigh wave speed c_R. However, this limit is frequently violated in rubber-like materials [1,2] and earthquake faults, presenting a fundamental paradox. We resolve this discrepancy by using an exact analytical solution for steady-state crack propagation in general linear viscoelastic solids using the Wiener–Hopf method [3]. Our analysis reveals that viscoelasticity replaces the classical Rayleigh limit with a universal speed limit: $V < \sqrt{\lambda}\, c_R$, where $\lambda = \mu_\infty/\mu_0$ is the ratio of high-frequency (glassy) to low-frequency (rubbery) elastic moduli. For typical elastomers where $\lambda \sim 10^2$–10^3, this permits crack speeds 10–30 times higher than the classical limit, enabling both intersonic ($c_\mathrm{s} < V < c_\mathrm{p}$) and supersonic ($V > c_\mathrm{p}$) propagation.

Method: We formulate the problem of a semi-infinite crack propagating in a two-dimensional viscoelastic strip under mode I loading. The constitutive relation for a general linear viscoelastic solid incorporates the complex modulus $\mu^*(\omega)$, which captures frequency-dependent material response. Using the Wiener–Hopf method, we derive closed-form analytical solutions for the displacement and stress fields. The energy release rate at the crack tip establishes the relationship between applied loading and crack velocity.

Results: The physical origin of the enhanced speed limit lies in the dynamic glass transition at the crack tip: rapid deformation rates cause the crack-tip region to experience the hard glassy modulus μ_∞, while the far-field material responds with the soft rubbery modulus μ_0. This modulus mismatch locally increases the effective wave speeds by a factor of $\sqrt{\lambda}$, creating conditions for supersonic propagation. Our solution predicts characteristic signatures of supershear propagation: (i) crack-surface oscillations in the intersonic and supersonic regimes, and (ii) Mach cone formation when crack velocity exceeds elastic wave speeds. In the intersonic regime, a single Mach cone appears with angle $\theta_\mathrm{s} = \arcsin(c_\mathrm{s}/V)$; in the supersonic regime, nested Mach cones emerge.

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Polydispersity as a control parameter for entanglement and packing in polymer solutions

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Polydispersity is ubiquitous in soft-matter systems, yet its quantitative role is often obscured by conventional metrics that fail to describe broad, non-Gaussian size distributions. In many polymeric and biological environments, molecular-weight distributions exhibit heavy tails, where minor components can dominate collective behavior [1, 2].

Here, we introduce a controlled experimental platform to investigate how continuous molecular-weight polydispersity governs polymer dynamics. Using polyethylene glycol (PEG) solutions with engineered power-law molecular-weight distributions spanning four orders of magnitude (see Fig.1a), we systematically vary the distribution exponent a while keeping fixed molecular-weight cutoffs. We identify an intermediate regime, $1 < a \lesssim 2.5$, in which the viscosity scaling exponent in the entangled regime, the overlap concentration c^*, and the entanglement concentration c_e all exhibit pronounced maxima exceeding monodisperse limits (see Fig.1b).

This amplification arises from competing effects of long and short chains: long polymers enhance entanglement and aggregation, whereas short polymers promote void filling and efficient packing (see Fig.1c). Notably, this regime coincides with the range of a where the mean and variance of the distribution diverge, highlighting the role of heavy-tailed statistics. These findings establish the power-law exponent a as a universal control parameter linking polymer entanglement, soft packing, and jamming-like behavior in highly polydisperse soft matter.

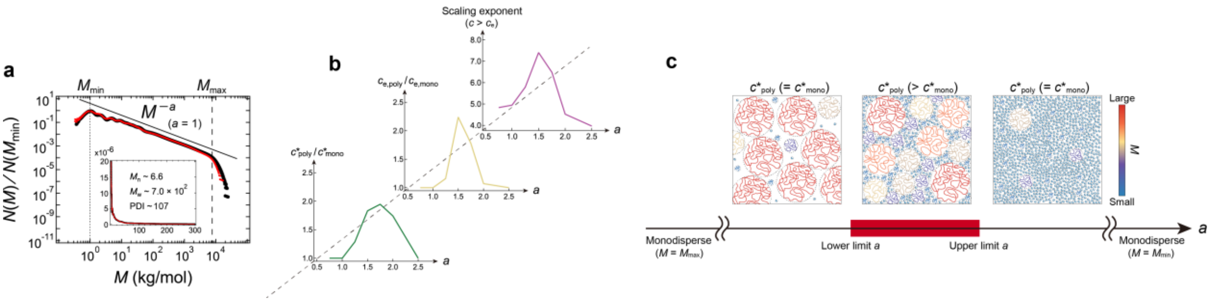

Figure 1: Schematic overview of the present study

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Characterizing polymer semiflexibility through structure factor and relaxation modulus measurement

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Multi-particle Brownian Dynamics simulations are employed to investigate the static and dynamic behavior of bead–spring chain models for semiflexible polymers and wormlike micelles. Semiflexibility, finite concentration, and additionally in the case of micelles, reversible scission generates a hierarchy of competing length and time scales. We demonstrate that Kratky representations of the static structure factor help to resolve key mesoscopic length scales—including the persistence length, correlation-blob size, and radius of gyration—each of which exhibit systematic scaling behavior with stiffness, concentration, and solvent quality. Rouse-mode analysis is used to quantify dynamic behavior, with the determination of the relaxation times that govern crossovers between bending-dominated and flexible-chain regimes. Furthermore, calculation of the relaxation modulus enables the identification of distinct viscoelastic regimes, such as the bending-to-flexible crossover, the concentration-dependent Zimm to Rouse transition, and sticker-mediated relaxation that is unique to micellar system. By linking static structure factor scaling, Rouse mode analysis, and linear viscoelastic response, this work provides a unified framework for identifying and interpreting the interplay of distinct length and time scales in semiflexible polymers and wormlike micellar solutions.

Dielectric Relaxation Studies on Poly(*N*-isopropylacrylamide) Microgel in a Water-Methanol Mixed Solvent System

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Aqueous suspension of non-ionic poly(N-isopropylacrylamide) (PNIPAM) microgel particles was synthesized via free-radical precipitation polymerization. On the synthesized PNIPAM microgel particles, a dynamic light scattering experiment was performed, and hydrodynamic radii were determined to be roughly 240 and 125 nm for temperatures of 25°C and 40°C, respectively [1,2,3]. Dielectric relaxation studies were carried out on a 10wt.% PNIPAM solution prepared in a mixed solvent system of 70% water and 30% methanol, and on the pure solvent mixture, over a broad frequency range of 100 MHz to 50 GHz and at temperatures between 5°C to 50°C. The dielectric spectra for the pure water-methanol mixture showed a dominant relaxation process associated with the collective reorientation of hydrogen-bonded networks. The relaxation for the polymer solution arises from (i) polymer-solvent coupling and (ii) the restricted dynamics of water molecules confined within the polymer network. Upon increasing the temperature, both samples show decreased relaxation times, implying faster molecular reorientation and a gradual weakening of hydrogen-bond interactions [3]. Figure 1 shows the real (ε′) and imaginary (ε″) parts of the dielectric spectra for the 10 wt.% PNIPAM microgel-solvent system. As the temperature increases, both ε′ and ε″ decrease, indicating reduced dipolar polarization and dielectric loss due. The relaxation peak in ε″ shifts toward higher frequencies with increasing temperature. The findings of this study will be presented.

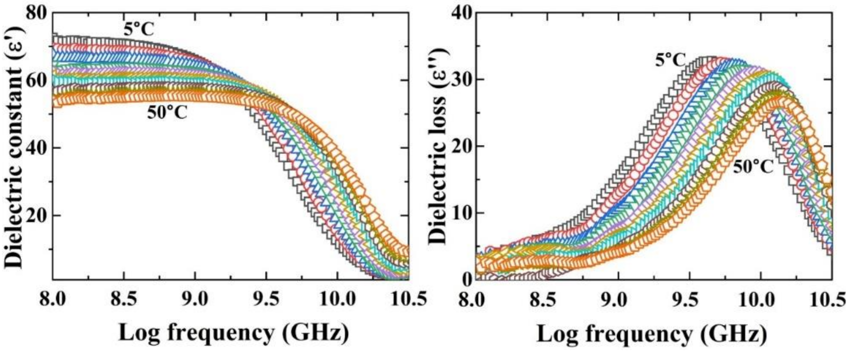

Figure 1: Real (ε′) and imaginary (ε″) parts of the dielectric spectra for the10wt% PNIPAM microgel in water-methanol mixed solvent from 5°C to 50°C.

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PG-Oral-11

Computational Modeling and Experimental Design of Drug-Eluting Intraocular Lens for Glaucoma Treatment

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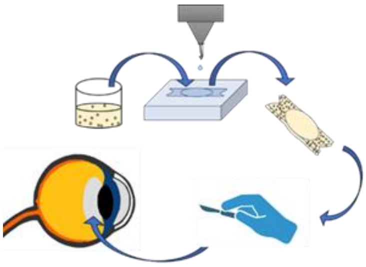
Eye drops suffer from challenges primarily associated with fast tear clearance resulting in poor drug bioavailability. The use of drug-eluting intraocular lenses may address this challenge by providing a sustained release of drug for prolonged periods. We present an in-silico modeling framework that can predict the spatiotemporal drug availability from the intraocular implants in the realistic anterio-posterior chambers of the eye. The model estimates the operational time period (defined as the duration for which the drug concentration at Trabecular Meshwork (TM) remains above the minimum therapeutic concentration level) of implant for different implant geometry and material properties of implant and drug. 3D simulations of intracameral implants reveal the effect of implant positioning and consequent spatial variations in drug concentrations at TM. We also explore two possible configurations of haptic implants – one with drug filled in a reservoir inside the haptic and another where the drug is uniformly distributed within the haptic. Next, we experimentally developed a drug-eluting Intraocular Lens (IOL) that ensures a sustained release of timolol (maleate) as an anti-glaucoma agent, for extended periods. Biodegradable Poly(lactic-co-glycolic acid) (PLGA) microspheres encapsulated with timolol are first synthesized using the water-in-oil-in-water (w/o/w) double emulsion method. These drug-loaded microspheres are incorporated in Poly(acrylamide–sodium acrylate) hydrogel (PAH) IOL cast from a 3D-printed mold, which is then monitored for sustained drug release for an extended period. Developed drug-loaded IOLs are transparent, flexible, and demonstrate sustained release of timolol for over 7 weeks. This release duration is drastically higher than direct drug loading in the PAH film, i.e., the degradation-control of drug release is much more efficient than drug transport by diffusion alone. Moreover, the incorporation of PLGA microspheres in the PAH film slows PLGA degradation, resulting in a 3-fold increase in release duration when compared to standalone microspheres. The resulting system ensures a long-term, patient-friendly approach for glaucoma treatment.

Graphical abstract



Discrete Knot-Core Sizes in Semiflexible Chains under Tension

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Knots in polymers are generally regarded as local objects in equilibrium, yet their quantitative behavior under external tension remains largely unexplored for semiflexible chains. In this work, we show that when a semiflexible polymer is tightened by force, the knot core enters a regime in which its characteristic size becomes discrete rather than continuously tunable.

We identify a physical mechanism underlying this behavior: as the knot core is tightened, internal configurational degrees of freedom become effectively frozen, rendering the entropic contribution to the free energy extensive while bending elasticity dominates. This leads to a topology-controlled selection of knot-core sizes that is insensitive to microscopic details.

We demonstrate the robustness of this mechanism using generic polymer simulations, oxDNA simulations of DNA knots, and macroscopic NiTi wire experiments in which thermal fluctuations are absent. Our results reveal a universal, geometry-controlled mode of knot tightening under force, with implications for both polymer physics and experimental identification of knotted structures.

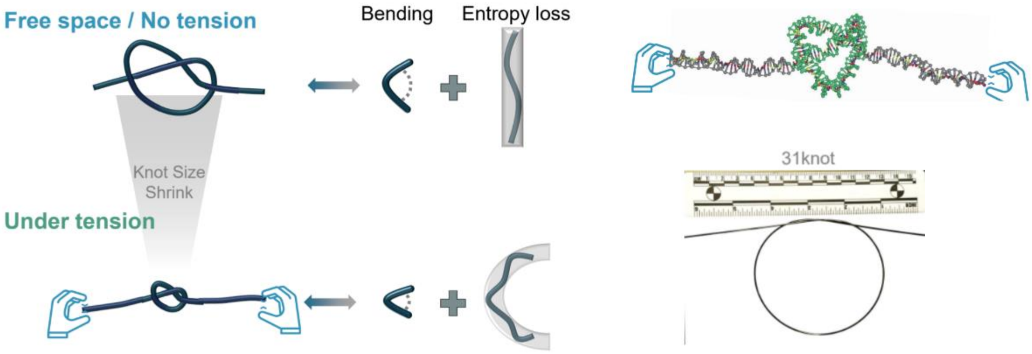

Figure 1: The free energy analysis for knot in free space and under tension. Illustration for DNA knot simulation and NiTi knot experiment.

[1] Qiyuan QIU, et al. *Discrete Knot-Core Sizes in Semiflexible Chains under Tension (2026) to be submitted*

Charged polymers: Gels, Kinetics, Intrinsically Disordered Proteins, Salt Effects

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Title: We shall present our work for last few years on charged polymers. Especially, we shall discuss our theoretical analysis of the swelling of polyelectrolyte gels in salt solutions, its application to drug delivery in biological conditions, intrinsically disordered proteins (IDPs) and its conformations in physiological solutions of monovalent and divalent salts, and also at different pH-conditions.[1]

[1] Chowdhury, Aritra; Borgia, Alessandro; Ghosh, Souradeep; Sottini, Andrea; Mitra, Soumik; Eapen, Rohan S.; Borgia, Madeleine B.; Yang, Tianjin; Galvanetto, Nicola; Ivanovic, Milos T.; Lukijanczuk, Pawel; Zhu, Ruijing; Nettels, Daniel; **Kundagrami, Arindam** and Schuler, Benjamin. 2023."Driving forces of the complex formation between highly charged disordered proteins." *Proceedings of the National Academy of Sciences*, 120, 2304036120
[2] Ghosh, Souradeep and **Kundagrami, Arindam**. 2024."Effect of counterion size on polyelectrolyte conformations and thermodynamics." *The Journal of Chemical Physics*, 160, 084909
[3] Ghosh, Souradeep; Chowdhury, Aritra; Tomares, Dylan T.; Schuler, Benjamin; Kundagrami, Arindam; Pappu, Rohit V.; 2025. "Interplay of distinct modes of charge regulation on poly-acid ionization and conformation" *The Journal of Chemical Physics*, 163, 194908
[4] A. Lastname, B. C. Lastname, *Phys. Chem. Chem. Phys.* **2023**, *1*, 234-240.

Ion Partitioning in Weakly Ionizable Hydrogels at High Ionic Strength

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Polyelectrolyte hydrogels can adjust their degree of ionization and redistribution of ions when they are in equilibrium with an electrolyte solution at a certain pH. This coupled ionization mechanism and partitioning behavior, governed by electrostatic interactions and Donnan potential, is important for understanding the swelling and ion uptake in such networks. But their behaviour in highly concentrated salt solutions and for complex charge patterns remains poorly understood. In this work, Using coarse-grained molecular simulations with the Grand-Reaction method[1], we study charge regulation and ion partitioning in cross-linked hydrogel networks modeled as weak polyacids with a pKa of 4.25, chosen to represent poly(acrylic acid) (PAA) in experiment, at high salt concentration close to the solubility limit. In the simulations, a cross-linked charged polymer network is equilibrated with explicit small ions and an ion reservoir using the simulation method, which is used to sample both acid-base reactions of the gel monomers and grand-canonical exchange of ions with the reservoir. The simulation results show how a change in pH and salt concentration influences the ionization degree of the gel, its swelling, and salt partitioning through changes in Donnan equilibrium and electrostatic interactions. For weakly acidic networks, simulation data indicate the expected increase of swelling of the gel and enhances ionization with increasing pH but reveal that at high salt concentration the Donnan partitioning of small ions is strongly suppressed and the gel loses its ability to establish a significant ion concentration difference relative to the surrounding solution. Experimental measurements on PAA hydrogels provide complementary data on swelling and ion uptake inside the gel, which are compared on a qualitative level with the simulation trends. This study is further extended to ampholyte hydrogel to understand how the positions of acidic and basic groups in the network further modifies charge regulation and salt partitioning[2].

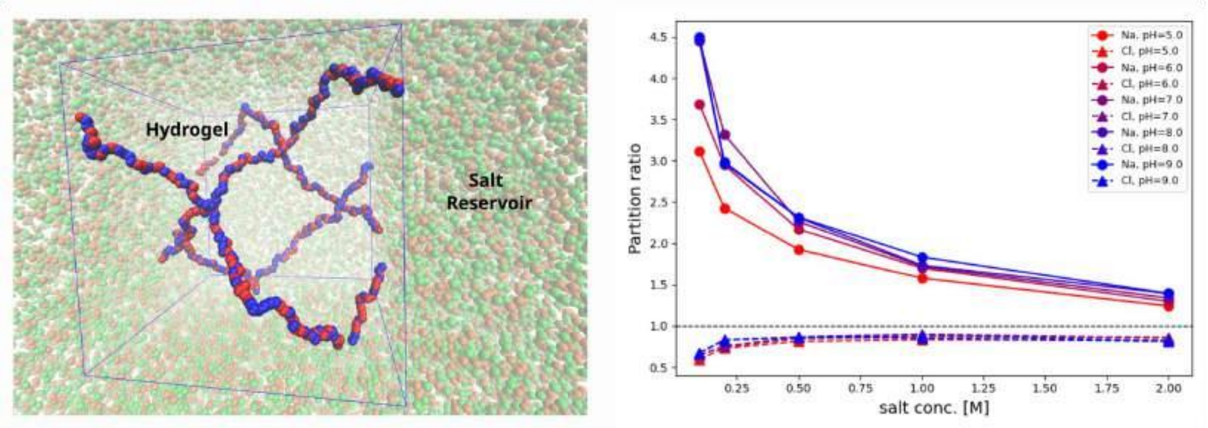

Figure 1: Snapshot of the modeled system with a plot of partition ratio of small ions

[1] J. Landsgesell, P. Hebbeker, O. Rud, R. Lunkad, P. Košovan, C. Holm, *Macromolecules* 53/8, 3007–3020 (2020)
[2] D. Beyer, P. Košovan, C. Holm, *Macromolecules* 55/23, 10751–10760 (2022)

Study of shear-induced behavior of nanocomposite hydrogels using molecular dynamics simulations

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Nanocomposite hydrogels (NCHs) overcome the mechanical limitations of conventional hydrogels by offering superior elasticity, toughness, and water retention – properties that enable geotechnical applications such as soil stabilization and frost resistance. In these contexts, understanding their response to shear is critical, as it governs flow behavior, energy dissipation, and network stability under deformations.

Here, we employ molecular dynamics simulations, with explicit solvent particles, to investigate the shear response of NCHs containing platelet-shaped clay nanofillers, under both charged and uncharged conditions. The nanofillers act as multifunctional crosslinking junctions that adsorp polymer chains, forming a percolating 3D network that enhances mechanical integrity. Our simulations reveal that increasing nanofiller concentration increases shear viscosity, leading to a gelation transition at 2.18% nanofillers. Upon application of shear, these NCHs display pronounced shear-thinning behavior, driven by nanofiller and polymer chain alignment along the flow direction. We further examine rheology, network connectivity, and structural orientation across varying shear rates, thereby providing molecular-level insight into the structure-property relationships of NCHs.

Transition Matrix Monte Carlo for tracking polymer conformations in explicit solvent

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Transition Matrix Monte Carlo (TMMC) algorithm is developed to compute the relative free energies of polymers in explicit solvents as a function of selected order parameter. We couple the polymer conformations in vacuum with explicit solvent environments using the Growth Expanded Ensemble. The method addresses the inherent sampling challenges in complex polymer systems by applying a bias in the simulation but computes the unbiased relative free energies. We demonstrate the method with a fully flexible polymer chain composed of Lennard Jones particles connected via a harmonic potential in solvent media. The relative free energies as a function of radius of gyration are computed for three different solvent qualities, created by changing polymer-solvent interaction strength. The results show a compliance with the theoretical predictions, that is, the polymer prefers extended conformation in good solvent and a collapsed structure in poor solvent. The proposed algorithm is flexible as it allows the creation of the polymer library using any simulation techniques such as Molecular Dynamics or Monte Carlo methods. It is capable of extracting the relative free energies at a particular system condition from the polymer library computed at different conditions thereby excluding the requirement of multiple simulations at respective conditions. The algorithm is adaptable to any collective variable (CV), can be extended to multiple CVs and scalable to parallel processing architectures. This computationally efficient framework to compute relative free energies have promising applications in polymer physics and larger molecular systems.[1]

Keywords: Transition Matrix Monte Carlo, Free energy calculations, polymer physics

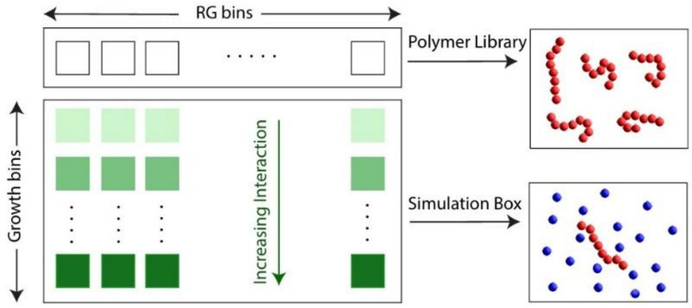

Figure: Transition matrix Monte Carlo to couple a polymer conformation in a vacuum with explicit solvent molecules via growth expanded ensemble.

[1] M. N. Angwani, K. Rane, *J. Chem. Phys.* 163, 014104 (2025).

On-Demand Reversible Crosslinks Enabling Sustainable All-Gel Supercapacitors

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The profound concept of dynamic reconfiguration is exemplified in nature through biological tissues, which eliminate old/damaged cells and regenerate new cells via bio-originating triggers and signals. This process ensures prolonged lifespans and adaptability to diverse environments. Despite being the best representative class of biomimetic materials, gels lack tissue-like reconstruction abilities. This is because the polymeric structures of most gels are inherently static, preventing them from undergoing molecular-level reconfiguration in response to artificial triggers/signals (1). The increasing utilization of these damage-prone synthetic gels with limited lifespans in applications including medical devices, soft robotics and stretchable or wearable devices, a trend forecasted to increase further, may synchronously contribute to substantial environmental waste, thereby necessitating immediate and sustainable solutions.

Inspired by the remodeling process of biological tissues, here we propose a glycerol-mediated supramolecular gelation strategy for reconfigurable gels. The reversible crosslinking structure of gel allowed on-demand reconfigurability in the presence of water, an environmentally friendly external trigger. Unlike synthetic gel, this gel offers reconfigurability and can be engineered for a wide range of functions and applications. We employed this strategy for developing gel electrodes and an electrolyte for a self-healable, degradable and reconfigurable all-gel supercapacitor (AGSC) (2). Notably the fabricated device exhibited a maximum areal capacitance of ≈450 mF cm^{-2} and cyclic stability of 89% after 20,000 charge-discharge cycles. Furthermore, AGSC demonstrated extreme environmental (-20 to 80 °C) and mechanical (stretching, bending and twisting) tolerance. This work opens routes for the development of a wide range of gel-based flexible devices with prolonging lifespan and recyclability, thereby reducing their environmental impact.

[1] A. V. Rama Varma, T. Das, Md. T. I. Mredha, T. Gupta, A. Raulo, D. Lee, W. Lee, S. Jung, M. Todo, I. Jeon, *Chem. Eng. J. 496, 153856 (2024)*

[2] Md. T. I. Mredha, A. V. Rama Varma, T. Gupta, I. Jeon, *Adv. Sci. 12, 2411847 (2025)*

10TH INTERNATIONAL SOFT MATTER CONFERENCE
(ISMC 2026)

Rheology and Non equilibrium Phenomena (RNP)

Understanding fluid flow using nonequilibrium molecular dynamics simulations

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The ability to predict and understand the molecular-level behaviour of fluids undergoing flow is increasing due to advances in experimental and computational approaches. These two approaches differ in the size-scales, time-scales and flow rates that can be directly probed as well as the ease with which molecule-level information, control of the structure, inclusion of realistic defects and reactive events can be achieved. From the experimental side, systems can now be probed at shorter length and timescales; with *in situ* and *in operando* analyses becoming viable. In contrast, computational hardware, software and new theoretical understanding have increased the length, timescales and complexity of systems that can be accurately simulated. However, there is still room for advances on both sides. In this presentation we discuss some recent nonequilibrium dynamics simulation studies that highlight current capabilities using computations at the molecular level. We will discuss how reactive events can be incorporated in simulations, the ability to simulate complicated systems with interfaces, and how we can combine ab initio calculations with nonequilibrium molecular dynamics simulations to predict viscosities. [1-3]

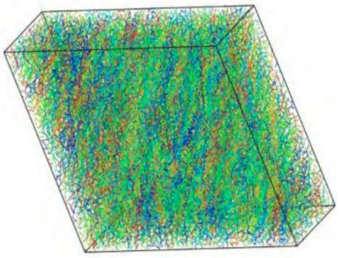

Figure 1. Configurations in a bulk polymer melt undergoing uniaxial extensional flow, obtained using nonequilibrium molecular dynamics simulations [1].

[1] M. Wang, S. Sanderson, D. J. Searles, *arXiv:2506.03945 [cond-mat.soft] (2025)*

[2] Z. Chen, Z. Yang, X. Tan, Y. Wang, B. Luo, X. Wang, M. Forsyth, C. J. Hawker, D. J. Searles, C. Zhang, *J. Am. Chem. Soc. 147, 31, 28464 (2025)*

[3] S. Sanderson, D. J. Searles, *arXiv:2512.01318 [cond-mat.soft] (2025), accepted*

Topological changes of local structure in dense colloidal suspensions under shear

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Understanding how microscopic structure controls the mechanical stability of glasses remains a central challenge in condensed matter physics. The local caging potential, arising from interactions with nearest neighbors, has emerged as a robust structural metric linking particle-scale structure to dynamics under thermal fluctuations and applied shear, yet its connection to specific local structural motifs remains unclear. We present a systematic analysis of local structural motifs in colloidal crystals and glasses and their correlation with the local caging potential. We show that polytetrahedral (icosahedral) motifs prevalent in glasses are associated with significantly deeper caging potentials than crystalline motifs such as face-centered cubic (FCC) and hexagonal close-packed (HCP) structures, while both crystalline and amorphous systems also contain a substantial population of stable defective motifs that play an important role in their mechanical stability. Under shear, clusters of defective motifs in colloidal glasses progressively fragment, driving plastic deformation and the transition from solid-like to liquid-like behavior, as particles escaping these clusters experience shallower caging potentials and undergo irreversible rearrangements. These results demonstrate that the loss of mechanical stability in amorphous suspensions is governed by the topological evolution of polytetrahedral motifs, revealing a clear structural mechanism underlying plastic deformation and shear-induced fluidization.

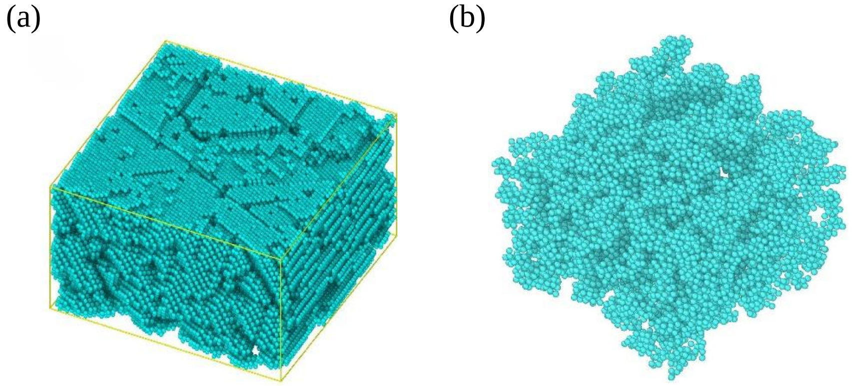

Figure 1: (a) FCC motifs in a colloidal crystal. (b) Defective icosahedral motifs found in dense colloidal glasses.

[1] Sahu, R, et al. "Shear induced topological changes of local structure in dense colloidal suspensions." *arXiv preprint arXiv:2508.15621* (2025).

RNP-Oral-02

Simulating turbulent polymer solutions using Brownian configuration fields

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Accurate simulations of turbulent polymer solutions are critical for applications of turbulent drag reduction. The complexity of the equations governing the dynamics of polymer solutions is, in significant measure, due to Brownian fluctuations, which through ensemble-averaging gives rise to a tensorial evolution equation for the polymer conformation [1]. If Brownian noise is disregarded, then the conformation equation would reduce to a vector equation for the polymer extension; apart from being far easier to simulate, a vector equation would allow finite extensibility to be enforced exactly [2]. Such a simplification seems reasonable in turbulence where flow fluctuations are expected to dominate over Brownian noise. We explore this possibility by simulating the vector or uniaxial model for a solution of linear dumbbells and comparing the results to the exact Oldroyd-B tensorial model; surprisingly, we find that Brownian fluctuations play a decisive role in preventing polymers from contracting irreversibly and being lost, while noise-free polymers tend to get depleted along Lagrangian trajectories that bypass or misalign with strain. We then derive successive corrections to the uniaxial model using Stratonovich calculus to incorporate noise only on the extension of the polymer, leading to a drift correction. Finally, to accurately simulate finitely-extensible dumbbells (without the Peterlin or similar closures), we use the full method of Brownian Configuration Fields (BCF) [1,3], employing several hundred fields to converge to the ensemble-averaged dynamics.

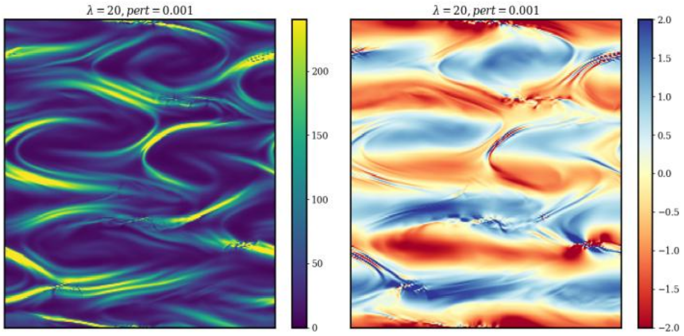

Figure 1: Uniaxial model polymer stretching (left) and vorticity (right) in Kolmogorov flow.

[1] Keunings, *Rheology Rev.* **2004**, 67-98 (2004).
[2] Fouxon and Lebedev, *Phys. Fluids*, **15** (7), 2060–2072 (2003).
[3] Mangoubi *et al.*, *J. Non. Newt. Fluid Mech.* **157** (3), 188-196 (2009).

Nonlinear rheology of unentangled polymer liquids: Insights from molecular simulations

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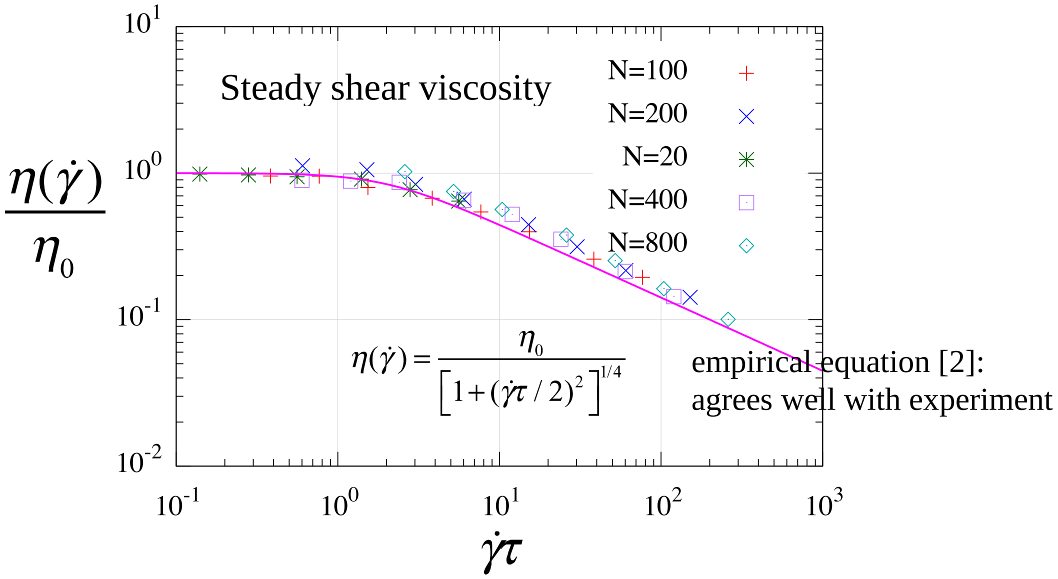
In the linear regime, the dynamics and rheology of unentangled polymeric liquids can be well described by the Rouse model. The model however fails spectacularly in describing phenomena observed under fast flows, such as shear thinning and stress overshoot. Therefore, we have performed extensive coarse-grained molecular dynamics simulations of unentangled polymer melts and solutions. The models used were: (1) standard Kremer-Grest model (short chains), (2) Rouse+XV model (Rouse-like model with strong excluded volume interactions between the different monomers), and (3) "soft core" models (weak excluded volume between the different monomers). As chain crossings were permitted in models (2) and (3), using them we could simulate long chains that did not exhibit any effects of entanglements.

The figure below shows the variation of the steady shear viscosity of unentangled polymer melts with the nondimensionalized shear rate obtained from models (1) and (2). While models (1) and (2) exhibited shear thinning in agreement with experiments, we found that the "soft core" models (3) showed very weak shear thinning (not shown). This suggested that excluded volume interactions, which are believed to be effectively screened in melts, are crucial for the observation of shear thinning under steady shear flow. The results of the simulations will be discussed from two perspectives: (a) flow-induced molecular friction reduction [1 and references therin]; (b) shear blobs [2,3]. I will argue that both of the perspectives are incomplete as each one can explain only certain of the observations. However, they can be thought of as being complementary in the sense that together they can account for all of the observations at hand.



[1] Watanabe et al., *Macromolecules* ***54****, 3700 (2021).*

[2] Colby et al., *Rheol. Acta* ***46****, 569 (2007)* .

Consistent non-equilibrium thermodynamics approach for rheological processes

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Theoretical description of rheological processes shows a variety of the approaches that address a rich nature of the complex fluids involved in non-equilibrium transformations. As such fluids show highly non-local and non-linear behaviour, classical non-equilibrium thermodynamics [1] fails to address them properly. Among the fundamental concerns that comes with this behaviour is apparent violation of the second law of thermodynamics. One of the approaches that overcomes this issue, known as Extended Irreversible Thermodynamics [2], employs non-equilibrium fluxes as independent variables, in addition to classical equilibrium variables (such as the density or the temperature). In effect, this rejects the hypothesis of local equilibrium but keeps the second law of thermodynamics intact.

In this talk I propose an alternative approach, that preserves the second law of thermodynamics and does not reject local equilibrium hypothesis [3]. Using the rates of change rather than fluxes, as the additional independent variable, I derive a consistent set of thermodynamics relations that govern a range of complex rheological processes [4].

[1] S. R. de Groot, P. Mazur, *Non-Equilibrium Thermodynamics; Dover: New York, 1984.*

[2] D. Jou, J. Casas-Vázquez, G. Lebon, *Extended Irreversible Thermodynamics*; *Springer, 2010.*

[3] K. Glavatskiy, *Entropy 27, 100 (2025).*

[4] K. Glavatskiy, *In preparation (2026)*

FIBRed fibres: Flow-induced bending response rheometer to measure bending of hydrogel microrods

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Microscale hydrogel fibers and rods play an important role in drug delivery, soft robotics, and tissue engineering. Their viscoelastic properties, stemming from the polymeric microstructure, are critical to their function, but they are often challenging to characterize. Conventional bulk tests - such as shear rheology or dynamic mechanical analysis - are often impractical for microscale fibrous materials because they are too small for standard equipment and difficult to manipulate in a controlled way. Here we introduce a flow-induced bending response (FIBR) rheometer that measures the bending modulus and viscoelastic properties of small, hydrated fibers and rods by using flow within a glass capillary. The fiber is placed across the capillary entrance, where pressure-driven water flow applies a quantifiable force to it. Fiber deflection is measured by video microscopy alongside the flow-rate data. We develop an analytical model to determine the hydrodynamic forces on the rod using the Rotne–Prager–Yamakawa approximation and apply Euler–Bernoulli beam theory to extract its material properties. We demonstrate the technique's versatility on natural and synthetic materials with diameters from 1 to 500 microns and elastic moduli from 100 Pa to over 100 MPa. The theoretical model describes both very slender fibers and thicker structures, the width of which becomes comparable with the size of the capillary. The presented method offers a flexible platform to characterize microscale mechanical properties of elongated structures [1].

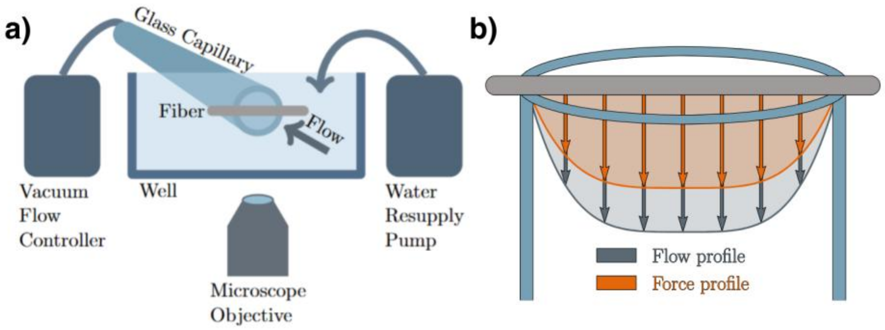

Figure 1: Schematic of the FIBR rheometer - a vacuum pump draws fluid through a capillary tube, causing the mounted fiber to deform; By analyzing the deformation under known flow conditions, we can determine bending modulus.

[1] B.T. Smith, M. Czerepaniak, M. Lisicki, S.M. Hashmi, *submitted* (2026).

Stretching of polymers in turbulence: effect of hydrodynamic interactions

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Polymers dissolved in a turbulent flow experience intermittent fluctuating strain-rates and thereby stretch and recoil repeatedly [1]. In this talk, I will examine the effect of intramolecular hydrodynamic interactions (HI) on the dynamics of stretching, using a hierarchy of models for the polymer and the flow—from dumbbells in a random velocity field to chains in a turbulent DNS [2]. Now, while HI have long been known to strongly affect polymer stretching in laminar viscometric flows, their role in turbulent flows remains unclear. Here, we show that HI-endowed chains exhibit a steeper coil-stretch transition as the elastic relaxation time is increased, i.e., HI cause less stretching of stiff polymers and more stretching of moderately to highly elastic polymers. On quantifying the repeated stretching and recoiling of chains by computing persistence time distributions, we find that HI delays migration between stretched and coiled states (Fig. 1). These effects of HI, which are consistent with chains experiencing an effective conformation-dependent drag, are sensitive to the level of coarse-graining in the bead-spring model. Specifically, an HI-endowed dumbbell, which cannot form a physical coil, is unable to experience the hydrodynamic shielding effect of HI [3]. Our results highlight the importance of incorporating an extension-dependent drag force in dumbbell-based simulations of turbulent polymer solutions.

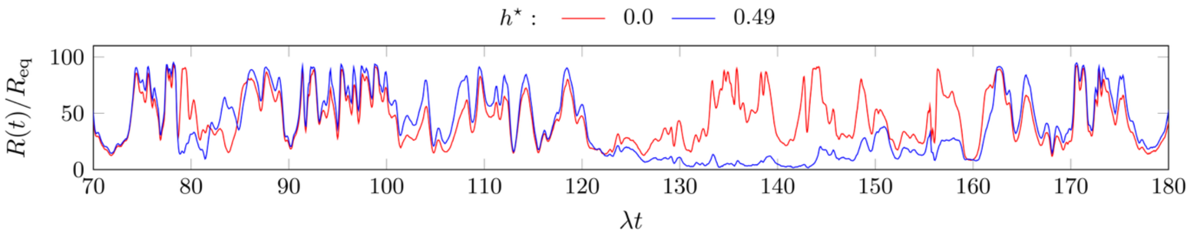

Figure 1: Typical evolution of the end-to-end extension of a bead-spring chain, without and with HI (h^* = 0 and 0.49, respectively), as it is transported in a homogeneous isotropic turbulent flow.

[1] J. R. Picardo, E. L. C. VI M. Plan, D. Vincenzi, *J. Fluid Mech., 969, A24 (2023).*
[2] A. Ganesh, D. Vincenzi, R. Prabhakar, J. R. Picardo, *arxiv:2509.05349 (2025)*
[3] J. R. Picardo, D. Vincenzi, *Phys. Rev. Fluids, 10, 093303 (2025).*

Tiny Movements, Big Changes: when the slow Arrhenius process decides how fast soft matter relaxes

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The properties of an ensemble at thermodynamic equilibrium do not change with time. Such conditions, however, are rarely encountered in nature. The transformation of buds into flowers and fruits, the rearrangement of tectonic plates on planetary surfaces, and the evolution of the human body over a lifetime illustrate systems operating far from thermodynamic equilibrium.
At the molecular level, equilibration kinetics—the time evolution of a system's properties toward lower-energy states—are directly linked to molecular motion. In accordance with Onsager's regression hypothesis [1], the macroscopic relaxation of a nonequilibrium system follows the same dynamical laws as spontaneous microscopic fluctuations under equilibrium conditions.
In simple liquids and soft materials, equilibration is typically governed by the α-modes, which control density fluctuations and whose characteristic timescales increase rapidly upon cooling. A growing body of experimental results suggests, however, the existence of an alternative equilibration pathway with a much weaker temperature dependence, characterized by a temperature-invariant activation barrier on the order of 100 kJ mol^{-1}.
We identify the molecular origin of this class of equilibration mechanisms with the slow Arrhenius process (SAP), detected by dielectric spectroscopy and related techniques [2]. The SAP is described within the collective small displacements (CSD) model [3], in which local amorphous packing is reorganized through molecular motions that are small in amplitude compared to those involved in the α-modes. By combining this picture with a statistical-mechanics-based equation of state capturing nonbonded segmental interactions, the CSD model predicts the SAP activation energy a priori based solely on thermodynamic material properties.
Finally, based on experimental findings on polymers and small molecules, we present a framework for soft material equilibration that provides quantitative predictions for technologically relevant processes, including polymer adsorption on silicon wafers [4] and crystal growth of small organic molecules in the glassy state [5].

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Small Steps, Big Impact: Understanding the protocol-dependent variations on gelation behavior

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Colloidal systems undergoing crosslinking have been of interest for several years due to their central role in the design of products and technologies across pharmaceuticals to cosmetics, coatings, and advanced materials. Although these gels provide a range of functionalities, their properties are often sensitive to processing conditions. In this work, we perform a study on Laponite® (a synthetic clay) dispersion and Pluronic solution to investigate the underappreciated yet critical role of preparation parameter and measurement protocols on gelation behavior of colloidal gels. We perform rheological experiments on the aqueous dispersion of Laponite® to monitor the effect of preparation parameters such as drying, stirring time, stirring speed, stirring technique, salt purity, sample volume, rheometer geometry, and ambient environmental conditions, on the gelation behavior. The aqueous dispersion of Laponite® unanimously exhibits all rheological signatures of sol-gel transition across multiple sample preparation protocols adopted in this study. However, the critical gelation time varies significantly upon change in the preparation parameters. Furthermore, we also monitor the thermoresponsive phase transition in polymeric solution upon heating and cooling. The transition temperature associated with liquid to soft solid state is observed to be influenced by both the rate of thermal cycling and the number of cycles applied. The findings of this work the advocate the importance of preparation parameter and measurement protocol in measuring the viscoelastic properties. The implications can be extended to a broad range of colloidal systems and offers a framework for more reliable characterization and efficient design of colloidal gels across disciplines.

Effect of pea-starch-hydrocolloids blending on pasting, linear and non-linear rheological characterization and decoding application specific functionality

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The present study investigated the effect of pea starch hydrocolloid mix blend ratio (r =0.9), which including pectin, chitosan, gelatin, guar gum, sodium alginate and whey protein isolate (WPI) on the paste formation, deformation behaviors, and application specific functionality. Comprehensive characterization of the mix blends on the pasting properties, 3ITT, small (SAOS) and large amplitude oscillation (LAOS), and creep were performed. Pasting studies reveled limited variation of peak temperatures-PT (66.7–70.2°C), although peak viscosity-PV (1229-7533 cp), break viscosity-BV (3.2-2832 cp), final viscosity -FV (2087-11300 cp) were mainly influenced by added biopolymers. Alginates and gelatin shows low BV values and set back values, indicating higher thermo-mechanical stability and reduced retro-gradation. In contrast, guar gum and pectin exhibits reduced PT values and significantly enhanced PV and FV, which enhance the water uptake, swelling of starch granules and responsible for amylose-gum network interaction. Whereas, chitosan and WPI evidenced mediate behavior with control swelling with structural integrity. Further, rheological analyses evidenced strong correlated with pasting behavior. The PS–WPI blends exhibited the highest breakdown ratio (62.3%) and thixotropic viscosity (~7.4×10^5 mPa·s), indicating strong shear-thinning but limited recovery (37.7%). PS–chitosan showed very high viscosity (2.16×10^6 mPa·s), moderate breakdown (36.6%), and good recovery (63.4%). In contrast, PS–guar gum displayed the lowest breakdown (19.7%) and highest recovery (80.3%), demonstrating exceptional structural stability and rapid rebuilding. PS–pectin formed a highly cross-linked but brittle gel ($G' \approx 5.4 \times 10^2$ Pa, $e_3 = -77$ Pa, $S = -0.66$), while gelatin and alginate blends exhibited moderate viscoelasticity ($\tan \delta \approx 2.5–4.7$), low breakdown, and improved thermal stability [1]. The obtained results suggest that pea starch functionality can be incisively tailored through biopolymer screen for flowable systems, 3D printing matrices, edible films, coatings, and soft gel based delivery applications etc.

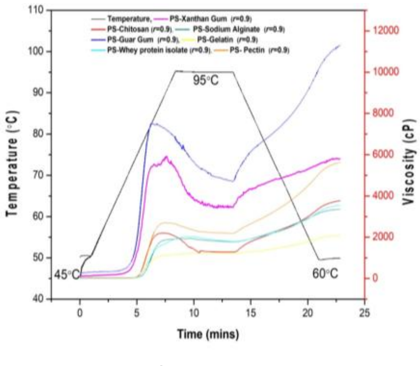

Fig 1: Pasting properties of Pea Starch blends mix ratio r (0.9)

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A Process Rheometer for Analyzing Flour Effects on Dough Sheetability

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Abstract

A study was carried out analyzing the effects of dough formulations (flour type and dough moisture) on dough rheology for a range of Australian and North American flours. Dough's rheological responses (elasticity and strain-hardening) were measured by rolling dough using an instrumented sheeter (1, 2). An apparent strain-hardening coefficient, which included elastic effects, was derived from roll forces and dough thicknesses obtained from sensors installed on the sheeter. Extensibilities of doughs were measured manually by measuring the end-to-end length of the pad at completion of sheeting. In parallel, portions of sheeted doughs were centrifuged to extract dough liquors. The volumes and viscosities of extracted dough liquors varied between flours and dough moistures. The apparent strain-hardening coefficient of doughs scaled linearly with changes in viscosity of dough liquor per unit volume of liquor, irrespective of amount of flour protein or growing region of wheat cultivars. The role of rheology of dough liquor on dough fermentation and crumb quality of breads(3) would also be discussed. The instrumented dough sheeter shows potential for rapid testing doughs for extensibility, strain-hardening and elasticity.

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Enhanced transport behavior of small molecules in polymer solutions

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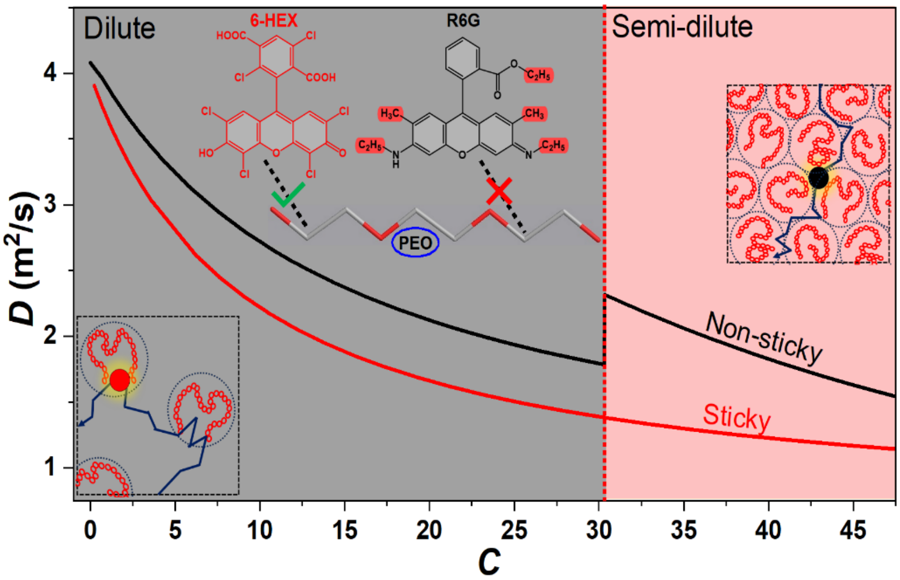
The transport of small molecules in crowded polymeric and biological environments is crucial for processes such as drug delivery and molecular imaging. Despite existing theories, anomalous transport behaviors persist. We report an unexpected increase in small-molecule diffusivity in aqueous polyethylene oxide (PEO) solutions near the dilute-to-semidilute transition. Using fluorescence correlation spectroscopy, we found that rhodamine 6G (R6G), a methylated dye, diffuses significantly faster than the non-methylated dye, 6-HEX, especially near the overlap concentration. Combining experiments with molecular dynamics simulations, we determined that molecular hydrophobicity affects transport. The hydrophilic dye adheres strongly to polymer chains, behaving like a "sticky" molecule, while the more hydrophobic dye interacts weakly. Simulations reveal the formation of regions with varying polymer density, which increases the volume of polymer-lean areas near the transition, facilitating the transport of non-sticky molecules. These findings challenge universal scaling models and highlight the significance of local heterogeneity and molecular chemistry in transport processes, offering new insights for molecular transport in complex environments.



Self Assembly and Self Organisation (SASO)

Programming Colloidal Self-Assembly for Advanced Materials

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Colloidal particles in the size range of hundreds of nanometers appeal as building blocks for photonic crystals with a complete photonic band gap in the visible [1]. However, the self-assembly of colloidal photonic crystals, which is touted as a low-cost, scalable fabrication technique, has proved elusive [2,3]. Diamond-structured colloidal crystals – much sought-after in their cubic form for a complete photonic band gap [4,5] – continue to remain challenging targets for scalable fabrication via programmed self-assembly [6,7], even after more than three decades of efforts. In this presentation, I will demonstrate, using a variety of computer simulation techniques, how hierarchical self-assembly pathways can be programmed and medium-range order can be encoded in designer patchy particles for facile self-assembly of colloidal photonic crystals [8-12]. I will highlight how certain long-standing challenges have been addressed to push the frontiers of colloidal self-assembly to develop a platform for advanced materials.

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Wave coarsening drives time crystallization in active solids

Corentin coulais

When metals are magnetized, emulsions phase separate, or galaxies cluster, domain walls and patterns form and irremediably coarsen over time. Such coarsening is universally driven by diffusive relaxation toward equilibrium. Here, we discover an inertial counterpart—wave coarsening—in active elastic media, where vibrations emerge and spontaneously grow in wavelength, period, and amplitude, before a globally synchronized state called a time crystal forms. We observe wave coarsening in one- and two-dimensional solids and capture its dynamical scaling. We further arrest the process by breaking momentum conservation and reveal a far-from-equilibrium nonlinear analogue to chiral topological edge modes. Our work unveils the crucial role of symmetries in the formation of time crystals and opens avenues for the control of nonlinear vibrations in active materials.

Vacancy defect delocalization dynamics in entropic crystals of Brownian squares

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Defects can readily form in entropically excited periodic structures in dense systems of hard-interacting particles since long-range interactions are absent; however, defect dynamics in these entropic crystals are not fully understood. I will discuss our experimental study of the dynamics of mono-vacancies, instantaneously created when a pulse of focused laser light ejects only a single particle, in two-dimensional entropic crystals, which have self-assembled rhombic and hexagonal symmetries, of hard colloidal Brownian squares. We show that mono-vacancies in entropic crystals become delocalized and migrate primarily along the crystalline lattice directions. The delocalization dynamics depend on complex stochastic collective effects, including the coupling between the translational and rotational diffusion of the squares. While the local configurational symmetry governs the available pathways for the propagation of excess entropy created by the mono-vacancies, the time scales for the progression of the entropy flow via delocalization depend on the particles' orientational ordering, which is imperative for their collective translational motion. This is in agreement with our earlier study demonstrating that the crystallization pathways in this system are solely governed by the orientational states accessible to the squares [1]. Our observations are further corroborated by Brownian dynamics simulations, which provide a local entropy map that can predict and elucidate delocalization dynamics.

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SASO-Oral-02

Complexity Lurking in Plain Sight: The Ubiquity of Lyotropic Dodecagonal Quasicrystals

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A delicate balance of noncovalent interactions drives hydrated molecular amphiphiles to self-assemble into aqueous lyotropic liquid crystals (LLCs) of varied topologies, with applications ranging from nanoporous separations membranes to mesoporous materials templates and therapeutic delivery vehicles. Spherical micelles are intuitively anticipated to form high-symmetry closest packed and body-centered cubic (BCC) LLCs. However, we recently discovered that ionic surfactant micelles also form a zoo of low-symmetry, tetrahedrally close-packed Frank-Kasper (FK) phases with spontaneously formed discrete micelle size distributions. The emergence of complex FK σ, A15, C14, and C15 LLCs arises from a frustrated non-covalent force balance that minimizes local variations in amphiphile solvation, while maximizing electrostatic cohesion in the ionic micelle ensemble. We describe how amphiphile structure and the path-dependent processing of their aqueous dispersions drive LLC sphere packing symmetry selection, culminating in our discovery of aperiodically ordered lyotropic dodecagonal quasicrystals (DDQCs) in three distinct amphiphile systems.

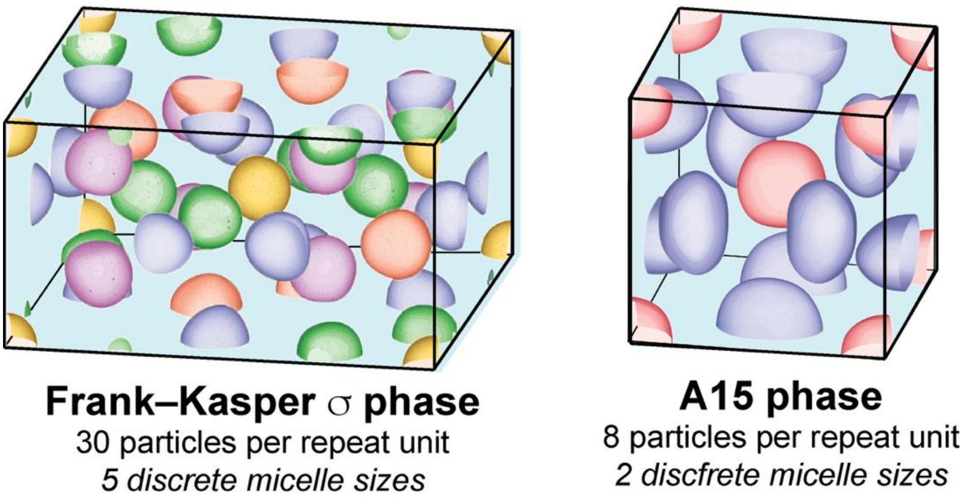

Figure 1: Electron density reconstructions of aqueous lyotropic Frank-Kasper σ and A15 phases, derived from self-assembly of simple ionic surfactants in water.

Tunable Active Droplet Assemblies

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Pattern formation occurs in diverse non-equilibrium systems. In biological environments, self-organization may occur when individual, motile agents interact with their neighbors via physical and chemical means. Inspired by nature, we seek to experimentally recreate this organization with active droplets. In high surfactant concentrations, oil-water emulsions spontaneously self-propel driven by micellar solubilization.[1,2] These droplets are auto-chemo-repulsive, avoiding each other and the trail of filled micelles they leave behind.[3] Furthermore, in 2D their hydrodynamic interactions do not typically allow for stable cluster formation.[4] This generally repulsive nature of confined active droplets provides a major limitation in the types of patterns that can emerge from the active droplet system. Recently it has been shown that using a liquid crystal oil phase allows for experimental control via temperature, as the internal order of the droplet affects the solubilization and in turn dynamics.[5] By careful selection of the liquid crystal and surfactant, we present a new, externally inducible, attractive and repulsive interaction allowing access to new emergent patterns from the active droplet system.

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De novo Emergence of Metabolically Active Protocells

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A continuous route from a disordered soup of simple chemical feedstock to a functional protocell—a compartment that metabolizes, grows, and propagates—remains elusive [1, 2, 3], as current frameworks typically rely on external environmental scaffolding or pre-synthesized biological components [4, 5]. Here, we show that a homogeneous aqueous mixture of phosphate, iron, molybdenum salts, and formaldehyde spontaneously self-organizes into soft, distinct compartments. Driven by non-equilibrium dynamics, these structures act as active chemical crucibles, coupling their own physical growth to the generation of chemical complexity. These structures function as long-lived, metabolically active reactors, accumulating a diverse repertoire of organic molecules including many bio-molecular precursors over months of sustained activity. Furthermore, they generate internal structures that are themselves growth-competent, establishing a rudimentary mode of self-perpetuation. The striking morphological and chemical resemblance of these synthetic protocells to naturally occurring spherules in marine sponges [6] suggests that this mode of self-organization is a robust, physically determined property of transition-metal chemistry. Our work establishes the most minimal, testable route to protocell formation till date, demonstrating that the emergence of life-like spatiotemporal organization from simple chemical conditions is much more facile than previously thought and might even be a recurring natural phenomenon [7, 8].

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Entropic Trapping of Hard Spheres in Spherical Confinement

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Monodisperse spherical colloidal particles confined within emulsion droplets can crystallize into icosahedral clusters. Experimentally, it was observed that a few large colloidal particles added as defects preferentially migrate to the vertices of the icosahedral clusters. To understand this structure formation phenomenon, we simulate the confined self-assembly of hard spheres in the presence of a small number of larger particles. The results demonstrate that large spheres are significantly influenced by concentric shells of small spheres near the crystallization transition. Entropic forces drive the large spheres to the cluster surface, where they settle into free energy minima at the icosahedron vertices. Notably, the addition of twelve large spheres results in the formation of a perfect icosahedral frame. Free energy calculations via umbrella sampling are used to quantify this process and show that both the migration to the cluster surface and the trapping at the vertices with trapping strength of multiple k_BT results from free energy minimization. Moreover, our study reveals that the crystallization pathway and dynamics of large spheres are consistent across different systems, suggesting robustness of entropic trapping [1].

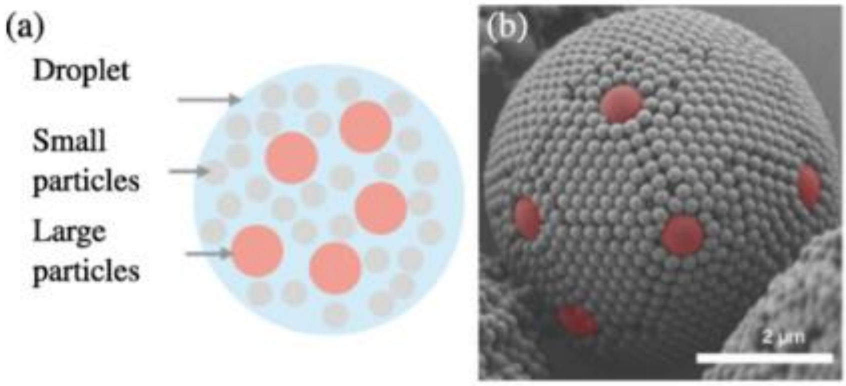

Figure 1: This is an image generated by ChatGPT

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SASO-Oral-06

Harnessing Dewetting Dynamics of Soft Thin Films for Nanoparticle Self-Assembly

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The self-organization of thin polymeric film like polystyrene occurs mostly because of instability caused by various reasons like van der Waals interaction, heterogeneous nucleation resulting in rupture and holes in the thin film. While most groups working in thin-films have found that incorporation of nano-particles have led to arresting of thin-film dewetting, our recent findings show that dewetting dynamics of the underlying thin-film can be used as a template that leads to the formation of unique self-assembled nano-particle patterns at the interface between graphene and a thin polystyrene (PS) film at room temperature. When a minute amount of NP dispersed in a solvent is added on PS and spin-coated into a thin film, the concentration gradient caused by centrifugal force leads to a Marangoni flow that in conjunction with the dewetting of the underlying PS at the edges lead to a series of very interesting and self-assembled morphologies of the nano-particles. At the particle enriched zone near the center, the graphene-particles exhibit morphologies ranging from folds, wrinkles, flakes, onion-rings to blob structures depending on the aspect ratio. The graphene-particles thrown to the periphery are found to march back towards the central portion leading to the unique formation of very ordered nano-scale scratches on the PS substrate. The graphene nanoparticles that end up into the confined rims in the intermediate region get twisted into nanoribbons and dendrimers [1]. When the graphene-PS system was replaced by CNT-PS system, CNT rings were found to encircle the dewetted zones [2]. Furthermore, applying this approach to nanoparticles of different physicochemical nature yields distinct morphological architectures; notably, iron oxide nanoparticles self-assemble into highly branched dendritic structures. The work sheds light on the forces responsible for the evolution of different origami structures formed as a result of the underlying dewetting dynamics without the aid of any high-end instrumentation. Since these self-assembled structures are formed over a biocompatible polymer, the structures are anticipated to find applications in fabricating biosensors, super-capacitors, and biomedical microfluidic devices.

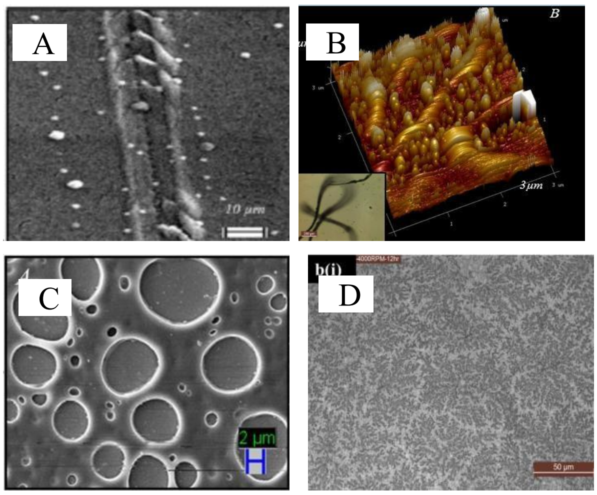

Figure1: (A) Nano-scale scratches of Graphene on PS films (B) NPS get twisted into nano-ribbons (C) CNT rings encircle the dewetted zones (D) Fe_3O_4 NPs form dendrimeric structures.

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Dynamics of complex molecular assemblies: What can we learn from atomistic computer simulations?

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Molecular self-assemblies have been on the forefront of research activities in several fields, most notably in the broad area of soft-materials science. Despite decades of effort, the fundamental underpinnings of the complex assembly processes and atomic resolution details of nano- and micron-scale assembled materials are poorly understood. Self-assembly is a multiscale process. The growth mechanism of single molecular building blocks dispersed in a solvent into higher order aggregates with well-defined morphologies typically involves complex spatio-temporal evolutions that defies simple explanations based on exiting theories. Our research group has been involved in an in-depth understanding of the origin of emergent complexity in molecular self- and co-assemblies using atomistic computer simulation methods. We used spontaneous assemblies of small peptides in water as model systems in our comprehensive atomistic simulation studies. We demonstrated that carefully crafted simulation studies, aided by automated analysis procedures for deciphering growth processes coupled with time dependent information of intermolecular interactions, could inform about the crucial early stages of the assembly covering the molecular to nanoscopic length-scales. We could establish clear relationships among the intermolecular interactions of the whole system, including solvation, the dynamics of the assembly and essential details of the morphology of the final assembled states. Free energy and rare event simulations and newly developed advance techniques provided quantitative assessments about key aspects of the assembly mechanisms. By systematic variations of the peptide sequence, we could explore the chemical space and understand the influence of molecular structure on assembly behaviors. Our analysis could explain why small changes in the structure of molecular building block lead to quite drastic changes in the outcome of the assembly – a somewhat puzzling observation often encountered in the field of molecular self-assemblies.

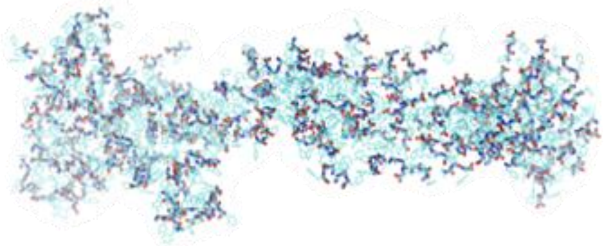

Figure 1: Atomistic picture of a spontaneously assembled 17 nanometer long tri-peptide nanofiber obtained from Molecular Dynamics simulation of the peptide-water system

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Fractal dimensions in patchy particle irreversible aggregation

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The fractal dimension of irreversible aggregating system gives information about the structure in the self-aggregating systems like colloids, proteins, etc. In this work, we performed a simulation study on the aggregation of spherical patchy particles interacting via four irreversible patches arranged in a square geometry along with a reversible isotropic square well potential. The structure formed have a fractal dimension close to reaction limited aggregation, whereas the local structure has hexagonal close packing. The structure factor calculation revealed that the presence of both mass and surface fractals. This was confirmed independently by calculating the mass fractal dimension from the cluster distribution. Calculating the surface roughness of the cluster revealed the presence of surface fractals, which varied with the strength of the isotropic potential.

Oscillatory Silica Precipitation and the Origin of Agate Banding

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During crystallization, quartz can assume various forms, giving rise to many minerals of scientific and aesthetic interest. One particularly captivating example is agate, a variety of chalcedony characterized by its rhythmic banding pattern composed of alternating layers with distinct colors. Despite extensive research efforts over many decades, the precise mechanisms responsible for agate band formation remain an open question. From a soft-matter perspective, agate offers a natural example of self-organized pattern formation in a silica-rich gel–fluid system that, during growth, behaves as a form of geological soft matter rather than as a rigid rock.

In this study, we introduce a phenomenological model to explain the formation of agate's rhythmic band structures, inspired by the work of Heaney and Davis [1]. In their model, rhythmic precipitation arises from self-organized oscillations in silica concentration at the mineral-solution interface, driven by competing processes of silica polymerization and diffusion-controlled transport. This interplay results in periodic changes in silica concentration, leading to the formation of distinct alternating layers characteristic of agate.

By solving the diffusion equation with appropriate boundary conditions, we show that the concentration at the growing interface undergoes periodic oscillations, which reproduce the observed banding patterns. We investigate how the wavelength of these oscillations depends on the physical parameters of the system and identify conditions required for their emergence. Building on findings from [2], we provide an analytical description of the concentration variations at the growing interface, and compare it with results of numerical simulations. Furthermore, we compare our model with other existing explanations for the creation of similar band structures in nature [3]. These results can serve as a basis for understanding how physical and chemical parameters influence the development of rhythmic banding, and offer a simple framework for interpreting the conditions under which such patterns may arise during agate formation.

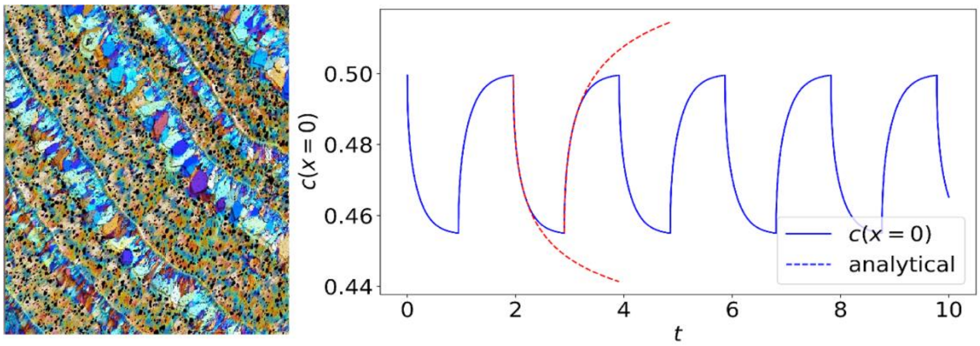

Figure 1: (left) Image of bands in an agate under optical microscopy; (right) numerically obtained concentration at the wall as a function of time (continuous line), compared with the analytically derived result for the same system parameters (dashed line)

[1] P. J. Heaney, A. M. Davis, *Science 269, 1562-1565 (1995)*

Sustainability (S)

The Art of Network Design

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We discuss several methods for designing polymer networks and gels, as well as various approaches to making these networks tougher, including the use of stored length and sacrificial bonds, slide rings, entanglements, and microphase separation. It turns out that whether weaker or stronger crosslinks lead to tougher networks depends on the placement of these crosslinks – either as parts of network strands or as connections between primary chains. The optimal strength of the sacrificial crosslinks and their concentration depend on the strength of the primary chain bonds. An interplay between main chain pull-out and bond cleavage depends on the deformation rate. A combination of these approaches in double networks utilizes double microphase separation on two different scales. All these methods lead to the narrowing of the tension distribution in network strands and, most importantly, the reduction of tension in the overstretched strands.

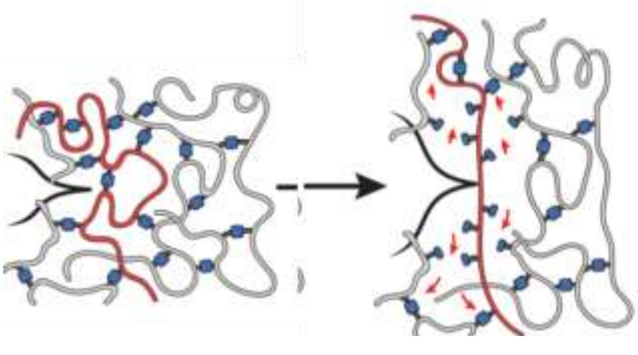

Figure 1: Weak interchain bonds make networks stronger [1].

[1] S. Wang, Y. Hu, T. B Kouznetsova, L. Sapir, D. Chen, A. Herzog-Arbeitman, J. A Johnson, M. Rubinstein, and S. L Craig, *Science, 380, 6651, 1248-1252 (2023).*

S-Oral-01

Cellulose swelling, gel formation and dissolution in Zwitterionic liquids

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Direct dissolution of cellulose in zwitterionic liquid (ZIL) is a multiple step process from wood pulp swelling, gel formation and viscoelastic polymer solution. The heterogeneous mixture of cellulose, water, and ZIL undergo changes as the water is gradually removed from the solution to form a solvated solution of cellulose in ZIL. This study deals with phenomena of material behavior during the transition of the plastic slurry of cellulose in ZIL, gel formation to viscoelastic biopolymer (dope). Dissolving grade cellulosic pulp and two (alkyl and oxyethylene) hexanoate based zwitterionic liquids were investigated for swelling, gel formation and dissolution studies. We examined the swelling and dissolution behavior of dissolving-grade pulp in an aqueous ZIL, specifically 1-carboxyhexyl-3-butylimidazolium and 6-(1-(2-methoxyethyl) imidazol-3-io)-hexanoate and compared it with *N*-methylmorpholine-*N*-oxide (NMMO), along with the rheological characteristics of the resulting cellulose solutions. Swelling and gel formation represents a critical pre-dissolution step, governing solvent diffusion into the fiber wall, disruption of inter- and intramolecular hydrogen bonding, and subsequent chain disentanglement.[1] The extent of swelling and dissolution kinetics of cellulose in two ZILs and NMMO solvent systems were systematically evaluated, and their influence on cellulose solution viscoelastic behavior was analyzed. The swollen cellulose samples were characterized for crystallinity and surface morphology. Rheological analysis revealed that cellulose solutions in both ZIL and NMMO exhibit viscoelastic behavior; however, at comparable cellulose concentrations, the ZIL-based dope showed significantly higher viscosity than the corresponding NMMO dope. These results provide insights into solvent–cellulose interactions that control swelling, gelation behavior and cellulose solution rheology, which are key parameters for cellulose processing and fiber spinning applications.

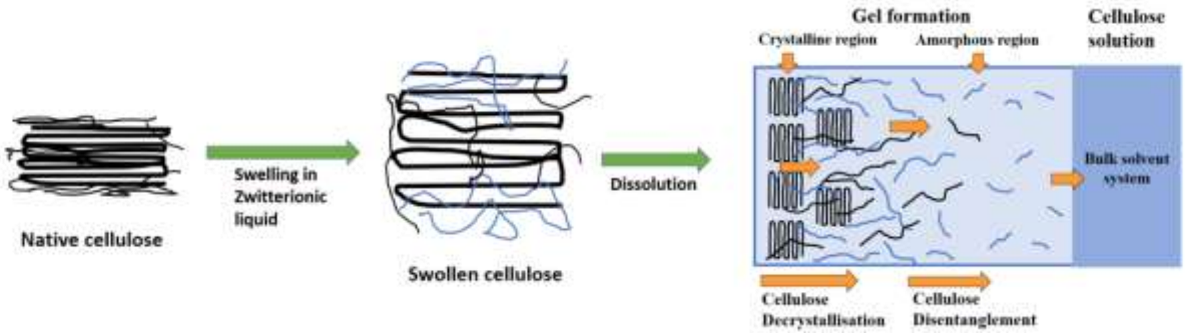

Figure 1: Process of cellulose swelling and dissolution in an aqueous zwitterionic liquid.

[1] B. Medronho, B. Lindman, *Current Opinion in Colloid & Interface Science, Volume 19, Issue 1, 2014, Pages 32-40, ISSN 1359-0294, https://doi.org/10.1016/j.cocis.2013.12.001.*

Chitosan Films Incorporated with Mango Leaf Quantum Dots for Packaging and Food Coatings

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The increasing accumulation of plastic waste, which contributes to global warming and health concerns, has led to a heightened demand for sustainable, home-compostable packaging solutions. This study investigates the use of dried mango leaves, processed into quantum dots as reinforcement, and chitosan derived from crustaceans as the matrix, to develop eco-friendly and functional packaging materials and food coatings. Chitosan films incorporating varying concentrations (1, 2, 4, and 10 wt%) of mango leaf quantum dots were fabricated using the solvent casting method. The morphology and structure of these films were characterized using Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), Small Angle Neutron Scattering (SANS), Fourier-transformed infrared spectroscopy (FTIR), and X-ray Diffraction (XRD). Mechanical, rheological, thermal, barrier, and surface properties were systematically evaluated. Additionally, functional properties such as antioxidant activity, soil biodegradability, and phytotoxicity were assessed.

Real-time monitoring of the developed coatings was conducted on eggplant and banana. Packaging films and food coating chitosan solutions containing mango leaf quantum dots (QDs) produced strong and flexible chitosan films with exceptional UV blocking efficiency (99.82%), enhanced thermal stability, high DPPH radical scavenging activity (95.2%), and extended the shelf life of banana and eggplant by more than 12 and 16 days, respectively.

Reprocessing of Semicrystalline Polymers via Directional Crystallization

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Directional crystallization (zone annealing) involves translating bulk material over a controlled thermal gradient, allowing melting and subsequent solidification [1]. Recent efforts on the directional crystallization of semicrystalline polymers (poly(ethylene) oxide (PEO) and its miscible blends) report preferential orientation of the crystallizable component along the imposed temperature gradient [2]. This process generates unique semicrystalline morphologies with stacked, uniaxially oriented crystalline (PEO) lamellae with amorphous interlayers. In this work, we aim to understand the roles of zone-annealing processing conditions, specifically the translational velocity and applied thermal gradient, as well as intrinsic material properties, such as polymer crystallization kinetics (nucleation and growth), on the resulting morphologies. These zone-annealed samples exhibit unique material properties, such as a direction (morphology)-dependent mechanical response. These results highlight the potential of non-equilibrium reprocessing of semicrystalline polymers to control the final structure and resulting properties through directional crystallization – a promising pathway for reprocessing commercial multi-layered semicrystalline polymers/plastics.

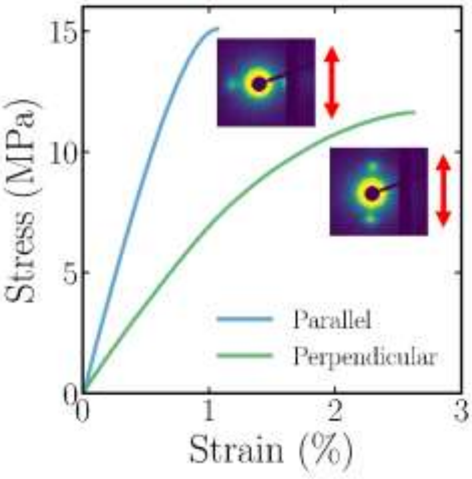

Figure 1: Mechanical response of zone annealed pristine PEO. Direction of applied stress with respect to the oriented crystalline lamellae shown in red.

[1] Lovinger, A. J.; Gryte, C. C, *Macromolecules, 9, 247–253 (1976)*

[2] Krauskopf, A. A.; Jimenez, A. M.; Lewis, E. A.; Vogt, B. D.; Müller, A. J.; Kumar, S. K., *ACS Macro Letters, 9, 1007– 1012 (2020)*

S-Oral-04

Valorization of Lignocellulose from Pistachio Shells for Bioplastic Films

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Waste biomass derived from animal, plant, and microbial sources represents a sustainable and renewable feedstock for the development of value-added materials, supporting circular economy and green chemistry principles. Among plant-based agro-residues, pistachio shells are generated in large quantities yet remain largely underutilized despite their high lignocellulosic content, comprising approximately 30-55% cellulose, 20-32% hemicellulose, and 12-38% lignin. [1] In this work, pistachio shell biomass was valorized through the selective extraction of lignin using alkali (15% NaOH), organosolv (80:20 ethanol:water with HCl catalyst), and deep eutectic solvent (DES; choline chloride:oxalic acid:ethylene glycol) systems. These fractionation routes yielded lignin with distinct molecular structures and polarity, characterized by variations in β-O-4 linkages, aromatic content, and functional hydroxyl groups, alongside a cellulose-rich fraction for material fabrication (Figure 1). Following delignification, the cellulose fraction was isolated, bleached with H_2O_2 to enhance purity, and converted into nanocrystalline cellulose, which was subsequently employed to fabricate mechanically robust cellulose films serving as a versatile platform for lignin incorporation. The incorporation of lignin obtained from different extraction routes enables modulation of film surface wettability while imparting multifunctional properties such as UV protection, antioxidant activity, and enhanced mechanical performance, with suitability for bulk films, surface coatings, or multilayered architectures. Overall, this integrated valorization strategy demonstrates the potential of pistachio shell waste as a renewable resource for sustainable packaging and soft-matter applications.

Figure 1: Schematic representation of pistachio shell biomass valorization, illustrating lignin extraction via different routes, cellulose purification, and bioplastic film formation.

[1] E. Robles, N. Izaguirre, A. Martin, D. Moschou, J. Labidi, *Molecules, 26, 1371 (2021)*

Understanding and Design of Sustainable Polymers

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Permanently crosslinked polymers are extensively used due to their favorable mechanical properties. However, these materials are unsustainable since they cannot be reprocessed. In contrast, polymer networks that can rearrange their topology without depolymerization, e.g., via the formation of reversible crosslinks, are reprocessable, and hence are promising candidates for a circular economy. The dynamic bond exchange in polymers is facilitated by reversible chemical reactions, such as transesterification or disulfide bond exchange, which enable favorable mechanical, rheological, self-healing, adhesive, and shape memory properties. Advancing the design of such sustainable materials requires a molecular-level understanding of how dynamic covalent networks regulate processability, recyclability, stress relaxation, and overall mechanical performance. We perform multiscale simulations and machine learning to accelerate the design of reversibly crosslinked polymers by linking bond-exchange kinetics, network topology, and macroscopic properties. We conduct density functional theory (DFT)-based electronic structure calculations to elucidate the bond-exchange kinetics in this class of materials. Moreover, grand canonical Monte Carlo (GCMC) and Molecular dynamics (MD) are combined to simulate and characterize viscoelastic behavior, stress relaxation, and the influence of crosslink structure on network dynamics. Machine learning models trained on simulation datasets enable the rapid prediction of key polymer network parameters, the identification of optimal monomer and crosslink chemistries, and the exploration of a broader design space with reduced computational cost. Together, this combined framework offers a predictive route for the rational design of sustainable polymer architectures with tailored functionality and enhanced circularity.

Reference:

(1) Karmakar, R.; Venkatareddy, N.; Himanshu; Valsecchi, M.; Maiti, P. K.; Sastry, S.; Kumar, S. K.; Patra, T. K. Computer Simulations of Entropic Cohesion in Reversibly Crosslinked Polymers. *Soft Matter* **2025**, *21* (3), 348–355. https://doi.org/10.1039/D4SM01161A.

(2) Karmakar, R.; Sastry, S.; Kumar, S. K.; Patra, T. K. Rouse Mode Analysis of Chain Relaxation in Reversibly Crosslinked Polymer Melts. *Phys. Chem. Chem. Phys.* **2025**, *27* (13), 6777–6785. https://doi.org/10.1039/D5CP00632E.

(3) Karmakar, R.; Chankapure, A. S.; Sastry, S.; Kumar, S. K.; Patra, T. K. Microphase Separation Controls the Dynamics of Associative Vitrimers. arXiv June 26, 2025. https://doi.org/10.48550/arXiv.2506.21066.

(4) Clarke, R. W.; Sandmeier, T.; Franklin, K. A.; Reich, D.; Zhang, X.; Vengallur, N.; Patra, T. K.; Tannenbaum, R. J.; Adhikari, S.; Kumar, S. K.; Rovis, T.; Chen, E. Y.-X. Dynamic Crosslinking Compatibilizes Immiscible Mixed Plastics. *Nature* **2023**, *616* (7958), 731–739. https://doi.org/10.1038/s41586-023-05858-3.

Application of Tulsi Modified Arecanut Fibre Bioplastic for Food Packaging

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The increasing problem of non-biodegradable plastic waste has driven the search for sustainable and eco-friendly alternatives in the food packaging industry. Simultaneously, the improper utilization of agricultural residues is contributing significantly to solid waste accumulation.[1] This research addresses these dual challenges by focusing on the development of an alternative to conventional plastic packaging while ensuring the efficient utilization of agricultural waste. This study reports the development of a bioplastic film using Polyvinyl Alcohol (PVA) as a biodegradable matrix which is reinforced with cellulose extracted from Arecanut Husk Fibre (AHF), and modified with Tulsi leaf extract as a natural antimicrobial agent. AHF is an abundant agricultural waste generated in India which contains a high cellulose content of 50.51%, making it a suitable reinforcement material for polymer composites.[2] The developed bioplastic composites were subjected to comprehensive characterization, including scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), mechanical testing, biodegradability studies, and antimicrobial evaluation. The results demonstrate that Tulsi-modified Arecanut fibre-based bioplastics exhibit significant potential as sustainable, value-added materials for food packaging applications.

Figure 1: Primary raw materials used for bioplastic film preparation: (a) AHF, (b) PVA resin, and (c) Tulsi leaves.

[1] Y. Lazim, S. M. Salit, E. S. Zainudin, M. Mustapha and M. Jawaid, *BioResources*, *9(4), 7721–7736 (2014)*

[2] C. L. Reichert, E. Bugnicourt, M.-B. Coltelli, P. Cinelli, A. Lazzeri, I. Canesi, F. Braca, B. M. Martínez, R. Alonso, L. Agostinis, S. Verstichel, L. Six, S. D. Mets, E. C. Gómez, C. Ißbrücker, R. Geerinck, D. F. Nettleton, I. Campos, E. Sauter, P. Pieczyk, and M. Schmid, *Polymers*, 12(7), 1558 (2020)

Deep eutectic solvent based 3D printable zein ink

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3D printing of materials allows rapid and cost-effective fabrication of complex geometries and customized features in product design. With increasing focus on sustainability and circularity, natural biopolymers have gained attention as eco-friendly alternatives for developing 3D printing inks. Among these, zein, a prolamine-rich protein derived as a by-product from the corn processing, is desirable due to its biodegradability, biocompatibility, and availability in large scale. However, native zein ink prepared in aqueous ethanolic solution suffers from poor printability, structural infidelity, nozzle clogging, and solvent evaporation, which significantly compromise their usability. In this study, deep eutectic solvents (DES) are used as a solvent to prepare zein inks for 3D printing applications. Rheological studies confirmed shear-thinning behaviour of the formulated eutectic zein inks with $\tan\delta < 1$, indicating a favourable viscoelastic profile for 3D printing. Optimized printing conditions for the formulated ink are found to be 20 mm/s speed, 90 kPa pressure, 45% infill, and 22G (0.41 mm) nozzle diameter. Further, the formulated inks exhibited improved performance, such as increased filament stability, reduced collapse, and enhanced structural integrity over the native zein inks. In addition to ink compliance for 3D printing, cell adhesion studies revealed excellent biocompatibility and fibroblast proliferation, underscoring the material's potential for biomedical applications. The findings of the study present a promising material formulation for sustainable and eco-friendly 3D printable bioinks in biomedical applications.

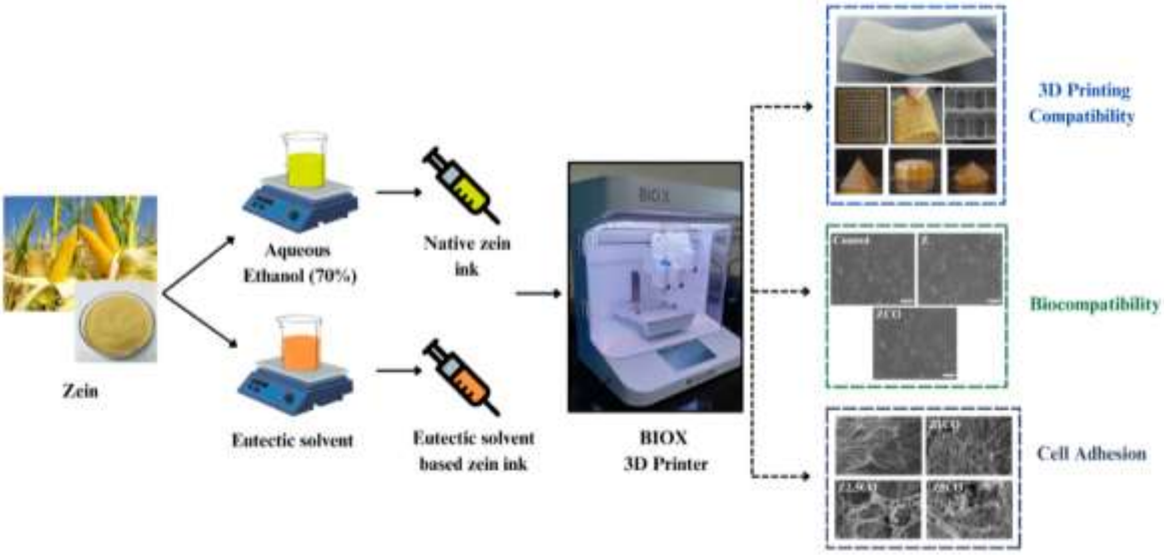

Figure 1: 3D printable zein ink

Accelerating Sustainable Soft Matter Discovery with Physics-Informed AI/ML

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Artificial Intelligence (AI) and machine learning (ML) are increasingly shaping sustainable soft matter and materials research, accelerating the discovery of functional polymers, complex fluids, and formulations with improved environmental performance. From recyclable polymers and bio-based materials to energy-efficient electrolytes and consumer product formulations, these tools enable faster and more informed design of sustainable soft matter systems.

But can AI/ML succeed without a foundation in physics and chemistry? Can we overlook decades of scientific understanding in favor of purely data-driven approaches? The answer is no. At Schrödinger, we combine physics-based simulations with machine learning built on chemically meaningful representations. This synergy improves accuracy, reduces experimental costs, and delivers insights even in data-limited scenarios.

In this talk, I will illustrate how Schrödinger's AI/ML approach supports sustainable materials R&D through real-world case studies. Our innovation operates on two levels: first, by improving the accuracy–efficiency trade-off in atomistic simulations via machine learning force fields (MLFFs), enabling high-throughput modeling of soft matter systems; and second, by directly applying AI/ML techniques to predict and optimize material properties relevant to sustainability, including durability, processability, and performance, in applications such as polymers, consumer goods formulations, and battery electrolytes.

S-Oral-09

Deep Eutectic Solvent-based Pickering Emulsions as a Green Platform for Biphasic Functional Materials

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While conventional oil-water emulsions are extensively studied, there is increasing interest in emulsion systems that do not include oil or water. Such non-traditional emulsions expand the scope of emulsion science and enable specialized, sustainable formulations for critical applications such as gas separation, CO_2 capture and drug delivery. In particular, deep eutectic solvents (DESs) have emerged as promising alternatives to conventional organic solvents due to their low toxicity, high thermal and chemical stability, negligible vapor pressure, tunable physicochemical properties, excellent solvation capabilities and easy synthesis.

Here, we report a new class of sustainable biphasic systems in the form of DES-based Pickering emulsions (PEs). Two distinct types of stable PEs are developed - (i) DES-in-silicone oil PEs and (ii) DES-in-DES PEs, both exhibiting tunable droplet sizes and dispersed phase loadings. The PEs are stabilized using functionalized nanoparticles and the approach is applicable for different DESs, including naturally available DESs (NADES). We further demonstrate the formation of high internal phase PEs (HIPEs) wherein the dispersed DES phase is encapsulated within a cross-linked outer shell composed of either silicone oil or another immiscible DES.

The large interfacial areas of these emulsions, coupled with the excellent solubilization capacity of DESs, make them attractive as functional materials for sustainable applications. To this end, DES-encapsulated sorbents are developed for CO_2 capture in both batch and continuous systems, showing promising CO_2 capture performance, good reversibility and robust structural integrity over multiple capture-release cycles. Overall, this work establishes DES-based emulsions as a scalable, green platform for next generation of CO_2 capture technologies.

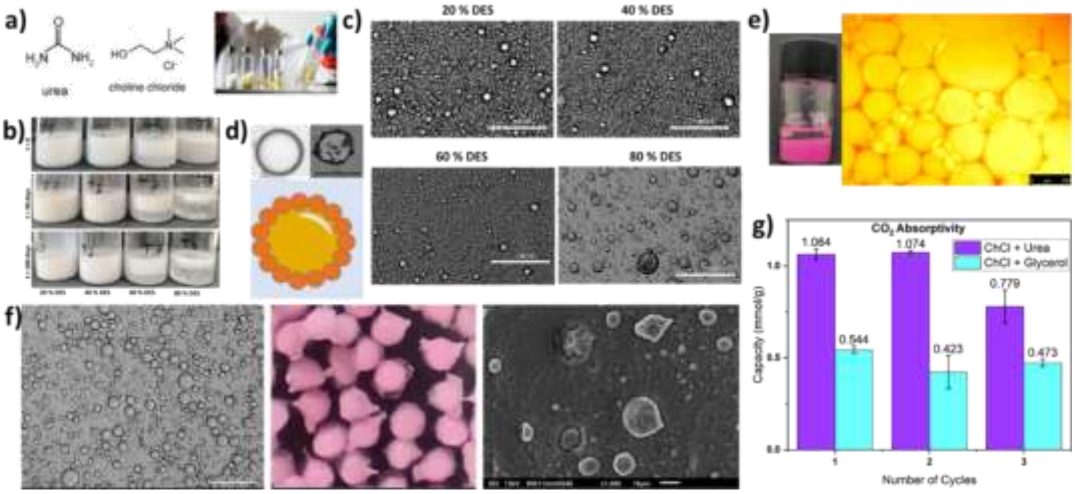

Figure 1. (a) Molecular structure of Choline chloride and Urea used to form a DES. (b) State of DES-in-silicone oil Pickering emulsions (20%, 40%, 60% and 80% DES v/v) after preparation (top) and after 6 months (below). (c) Optical micrographs of emulsions. Scale bars 100 μm. (d) Dark patches near the DES-silicone oil interface indicates the adsorption of TiO_2 NPs that have been functionalized with DMOAP and oleic acid. (e) DES-in-silicone oil HIPEs. (f) Vortex followed by crosslinking to prepare the DES-encapsulated sorbents. The hydrophilic dye, Bromothymol blue, was used to visually confirm the DES encapsulation. Scale bar 100 μm. SEM images of the prepared sorbents. Scale bar 10 μm. (g) CO_2 capture obtained from a batch setup using these sorbents