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Abstract Book

Oral Presentations

Plenary Talk Eugenia Kumacheva University of Toronto

Biomimetic fibrillar hydrogels: from mechanical properties to applications

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Man-made nanofibrillar hydrogels have emerged as a class of biomimetic materials reproducing the filamentous structure and properties of the extracellular matrix (ECM), acting as scaffolds for three-dimensional cell culture and tissue engineering, and offerring applications in sensing and soft robotics. The mechanical response of fibrous gels to strain is largely governed by the strong asymmetry in the deformation energy of the constituent filaments that are soft upon compression and stiff upon extension. This presentation highlights biologically relevant implications of such mechanical asymmetry.

In the first example, confinement of fibrous hydrogels in narrow capillaries mimicked obstruction of blood vessels with blood clots. We show experimentally and theoretically that filamentous gels respond to such confinement in a qualitatively different manner than gels formed by single-molecule flexible strands. Under strong confinement, fibrous gels exhibit a very weak elongation and an asymptotic decrease to zero of their biaxial Poisson's ratio. Such response results in strong gel densification and a weak flux of liquid through the gel. This behavior sheds light on the resistance of strained occlusive blood clots to lysis with therapeutic agents and stimulates the development of effective endovascular plugs for stopping vascular bleeding or suppressing blood supply to tumors.

The second example highlights the importance of structural anisotropy of fibrous hydrogels. For the filamentous synthetic hydrogel with a structure reproducing the organization of fibers in collagen networks surrounding cancer tumors, we show that the hydrogel's response to radial compression (replicating tumor growth) is governed by the type and degree of structural anisotropy of the gel network. These findings underline the importance of the design of 'precision biomaterials' that faithfully recapitulate key microenvironmental characteristics of cancer tumors.

Finally, an engineered nanofibrillar hydrogel has been designed as a scaffold for the initiation and growth of breast cancer patient-derived organoids, 3D cell cultures replicating the structure and function of cancer tumors. The hydrogel had highly controllable composition and mechanical properties. The organoids grown in the hydrogel had histopathologic features, gene expression, and drug response that were similar to those of their parental tumors, thus, offering a highly promising model for personalized medicine.

Plenary Talk Lucio Isa ETH Zurich

The Past, Present and Future of Capillarity-Assisted Particle Assembly (CAPA)

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The assembly of colloidal particles into targeted structures, clusters and arrays is at the core of many of the technologies, processes and materials that use micro and nanoparticles as their constitutive units. Among the different strategies that we have developed to direct colloidal assembly, the use of capillarity presents numerous advantages.

Capillary forces emerge whenever any colloidal particle deforms a fluid interface, are long ranged and can be orders of magnitude stronger than other colloidal forces. When combined with topographical templates, they can therefore be used to place different particles into prescribed patterns, from arrays of individual colloids to tailored multi-material clusters [1].

In this talk, I will present a brief historical perspective of Capillarity-Assisted Particle Assembly, or CAPA, followed by a review of where our group uses it and why. In particular, I will show that CAPA is uniquely suited to synthesize colloidal clusters, whose composition and geometry can be independently tailored to create a broad class of artificial microswimmers [2,3,4], and to template the nanoprinting of responsive hydrogels [5].

I will conclude by demonstrating that CAPA has still a lot to offer for the future, where overcoming some of its challenges has opened up new exciting opportunities. In particular, I will show how CAPA can be extended to the patterning and assembly of biological objects [6] and how, taking an icy twist, CAPA has now become even cooler.

Keywords: directed assembly, capillarity, colloids.

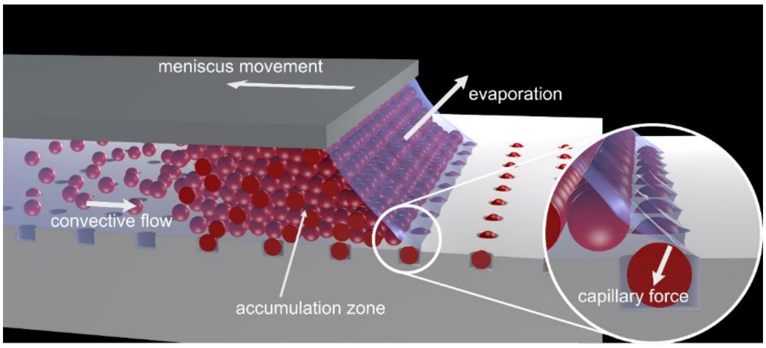

Figure 1. *Schematic of the working principle of capillarity-assisted particle assembly [1].*

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Plenary Talk Daniela Kraft Leiden University

Autonomous life-like behavior emerging in active and flexible microstructures

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Many organisms leverage an interplay between shape and activity to generate motion and adapt to their environment. Embedding such feedback into synthetic microrobots could eliminate the need for sensors, software, and actuators, yet current realizations at the micrometer scale are either active but rigid, or flexible but passive.

Here, I will show that 3D microprinting is a powerful tool to create anisotropic and flexible microswimmers.[1] I will discuss how shape affects their interactions and clustering behavior,[2] and introduce microstructures that integrate both activity and flexibility.[3] I will demonstrate that this minimal yet versatile design gives rise to a rich array of life-like modes of motion — including railway and undulatory locomotion, rotation, and beating — as well as emergent sense-response abilities, which enable autonomous reorientation, navigation, and collision avoidance.

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Plenary Talk Matthieu Wyart EPFL Lausanne

From the glass transition to creep flows

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Under cooling, a supercooled liquid undergoes a glass transition and stops flowing. Physicists do not agree on the microscopic reasons that make a glass solid. Some view this phenomenon as being collective in nature: it may be a signature of a thermodynamic phase transition, or being caused by kinetic constraints (where particles seek to solve a sort of Chinese puzzle). Others view it as simply reflecting elementary barriers for rearrangements, controlled by the elasticity of the material. To resolve this issue, I will introduce novel algorithm to systematically extract elementary rearrangements in a broad energy range. The analysis reveals that for simple glasses, relaxation is not cooperative in nature. I will then introduce a theory of dynamical correlations in super-cooled liquids based on coupled local rearrangements, which connects this phenomenon to avalanche-type responses observed in driven disordered materials. I will discuss positive empirical tests of this view in both realms, supporting that this framework unifies these different fields.

Transport dynamics of confined particles: from complex shapes to collective effects

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Understanding microparticle transport in complex environments is essential for applications ranging from pollution control to particle sorting and intracellular dynamics. Transport is governed by the interplay between particle properties, flow conditions, and environmental constraints, especially when particles have complex shapes or are present at high concentrations

Here, we investigate the transport of complex particles using microfluidic model systems. We first examine how particle shape influences transport dynamics in straight, confined channels, then explore the interactions of elongated particles with obstacles, which serves as a basis for analyzing fiber separation in pillar arrays. Finally, we address collective effects by studying the flow of gear-like particles through constrictions.

These findings offer new insights into the flow of complex particles in crowded environments, ranging from natural soils and the interior of cells to blood flow, and may enable advances in particle sorting and water treatment applications.

Plenary Talk Hajime Tanaka University of Tokyo

Network-forming phase separation in soft matter

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Phase separation is a fundamental process that governs the spatial organization of soft and biological matter. While conventional phase separation typically leads to droplet formation and coarsening via mechanisms such as Marangoni effects [1], an alternative pathway—viscoelastic phase separation (VPS)—can produce interconnected network or porous structures, particularly in systems with strong asymmetry in component mobilities, a common feature in soft materials [2,3].

In this study, we explore network-forming phase separation in colloidal suspensions and report a previously unrecognized coarsening law for VPS, where the characteristic domain size grows as $\ell \sim t^{1/2}$ [4]. In suspensions with short-range attractions, phase separation is often arrested, forming colloidal gels that retain mechanical stress—especially at low volume fractions—where the arrest is primarily mechanical rather than purely dynamical [2,3,5–8]. We also identify an alternative, stress-free gelation pathway, where a stable network forms without residual stress [9].

Furthermore, we examine the conditions under which self-similar coarsening emerges in VPS. Specifically, we explain its absence in uncharged polymer solutions [10] and its presence in complex coacervates, which are solutions of oppositely charged polymers [11].

These findings enhance our understanding of the physical mechanisms underlying network formation in phase-separating soft matter and provide new design principles for developing porous and field-responsive materials with applications spanning from materials science to biology [12].

Acknowledgements: This work was made possible through collaborations with Michio Tateno, H. Tsurusawa, Jiaxing Yuan, Shunto Arai, Mathieu Leocmach, and John Russo. This work was supported in part by Specially Promoted Research (JP20H05619) from the Japan Society for the Promotion of Science (JSPS).

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Monday 29th September 2025

A. Active matter

(Room 1)

Scale-free bacteria turbulence

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Fluids loaded with swimming micro-organisms have become a rich domain of applications and a conceptual playground for the statistical physics of "active matter" [1]. Such active bacterial fluids display original emergent phases as well as unconventional macroscopic constitutive properties [2,3], hence leading to revisit many standard concepts in the physics and the hydrodynamics of colloidal suspensions.

Here we show that above a critical concentration - scaling as the inverse of the vertical confinement- a suspension of active E.coli undergoes a hydrodynamic instability leading to a "turbulent-like" state characterized by a complex dynamics of vortices and jets (Fig.1a) [4]. The emergent structures and the temporal dynamics, scale over more than two decades, with the vertical confinement. Phenomenologically, the transition to active turbulence bears many similarities with a second order phase transitions limited by a spatial cut-off. We propose a finite size rescaling for both the correlations length divergence and the critical slowing-down dynamics that bring all our data onto a universal curve.

We also observe in the critical turbulent domain, the stochastic emergence of very large transient vortices (Fig.1b) which diameters can reach the lateral circular confinement. We bring evidences for a spatio-temporal dynamics resulting in a complex interplay between coarsening and fragmentation that remains up to now, unraveled.

Keywords : Active matter, Bacteria turbulence, Active suspensions

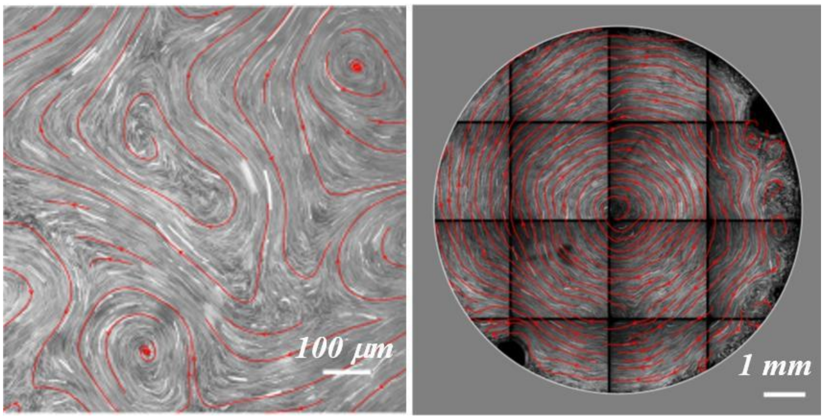

***Figure 1** – (a) Active turbulence state for a vertically confined droplet of E.coli suspension (H=630 μm), (b) also showing the emergence of a very large vortex state*

Acknowledgements: Grants ANR-22-CE30-"Push-pull" and H2020-MSCA-ITN-"Phymot".

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Locomotion of Active Polymerlike Worms in Porous Media

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We investigate the locomotion of thin, living *T. Tubifex* worms, which display active polymerlike behavior, within quasi-2D arrays of cylindrical pillars, examining varying spatial arrangements and densities. These active worms spread in crowded environments, with a dynamics dependent on both the concentration and arrangement of obstacles. In contrast to passive polymers, our results reveal that in disordered configurations, increasing the pillar density enhances the long-time diffusion of our active polymerlike worms, while we observe the opposite trend in ordered pillar arrays. We found that in disordered media, living worms reptate through available curvilinear tubes, whereas they become trapped within pores of ordered media. Intriguingly, we show that reducing the worm's activity significantly boosts its spread, enabling passive sorting of worms by activity level. Our experimental observations are corroborated through simulations of the tangentially driven polymer model with matched persistence length predicting the same trends.

Keywords: Active matter, Active polymer, Porous media, Transport.

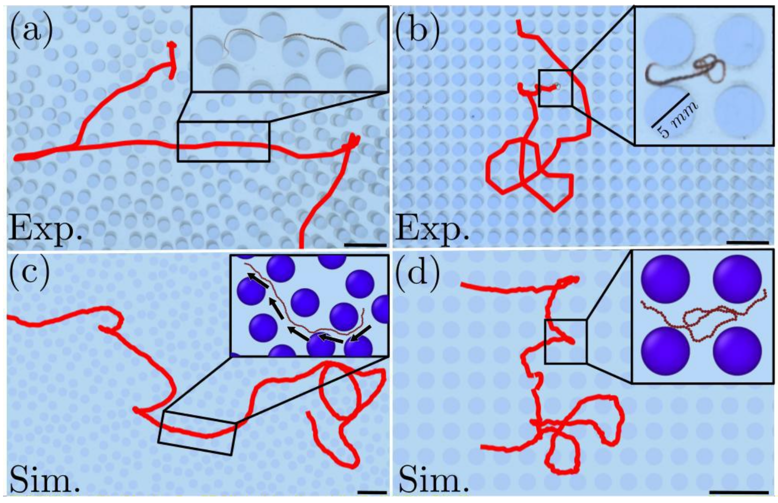

Figure 1. *Trajectories of the center of mass an active polymerlike worm in* $L^2 = 44 \times 44$ *cm*^{2} *2D array of pillars with a diameter of 5 mm and surface fraction* $\phi = 0.4$ *(only a part of medium is shown) in a (a) random packing and (b) square lattice for a duration of 185 s; scale bar corresponds to 15 mm. Close-ups show the distinct conformations of a worm arising in the two different obstacle arrangements. (c),(d) Center-of-mass trajectories and representative polymer conformations of the simulated tangentially driven active filaments in the same geometries as in (a),(b).*

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Unraveling the Mechanics of the FtsZ Ring during Bacterial Cell Division

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Cell division is a fundamental process in all living organisms, governed by complex biochemical and biophysical mechanisms. In bacteria, the tubulin-homologue FtsZ assembles into a tightly packed structure of individual filaments around the division site, called the Z-ring. This Z-ring recruits a multi-protein machinery responsible for peptidoglycan assembly and guides the inward growth of the rigid bacterial cell wall. However, it is still unknown how exactly the Z-ring remains precisely at the leading edge of the closing septum (despite its changing curvature) and whether or not it exerts an inward force on the inner membrane while doing so.

The defining feature of FtsZ is treadmilling, directional growth at one end and shrinkage at the other, leading to apparent filament motion while individual monomers remain stationary. We previously showed how the interplay of filament treadmilling and chemical patterning leads to a stable formation of the Z-ring around the mid-cell [1]. Here we present a coarse-grained, three-dimensional model of treadmilling FtsZ and apply it to coarse-grained cell wall models in molecular dynamics simulations.

We probe the interplay of FtsZ filaments' intrinsic curvature, cell shape and attractive forces mediated through binding proteins FtsA and ZapA on the positioning of the Z-ring. We then investigate the ability of these curved filaments to exert an inward force onto the inner cell membrane and stay in place as division occurs. Overall, we demonstrate our models' ability to capture experimentally observed filament behaviors [2] and elucidate the role of FtsZ in bacterial cell division.

Keywords: Cell division; FtsZ; Computational biophysics; Active matter

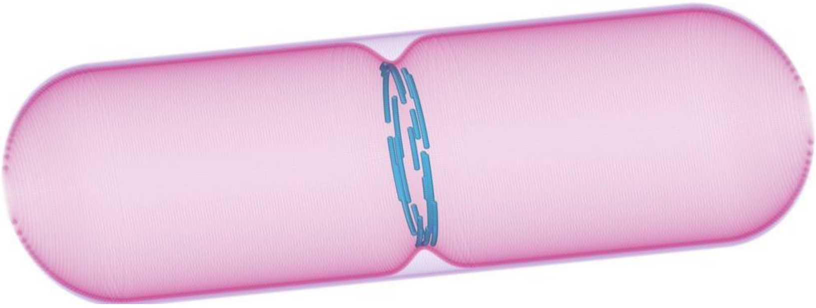

Figure 1. *Schematic of coarse-grained simulations of bacterial cell division. Treadmilling FtsZ (blue) on a closing membrane (pink) surrounded by rigid cell wall (purple).*

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Magnetic control of bacterial turbulence

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Dense suspensions of active agents exhibit various organized collective states not possible in equilibrium systems. A notable example is the hydrodynamic instability of pusher-type particles, which leads to an active turbulent-like state consisting of intermittent vortices and jets. Here we show that this active turbulence can be externally controlled by imposing aligning torque on the active agents mediated by a magnetic field and a magnetizable fluid. We demonstrate this for the case of bacterial turbulence using Bacillus subtilis 3610 in Terrific Broth medium that contains aqueous ferrofluid of PEGylated iron oxide nanoparticles. These nanoparticles do not attach to the bacteria and hence do not significantly alter their swimming characteristics but still provide the required magnetic contrast for torque generation.

At low bacterial concentrations, we observe gradual buildup of nematic alignment of the rod-shaped bacteria in horizontal magnetic field. Partial alignment appears already at very small fields, a few mT only, saturating at around 15 mT. In the saturated state, the bacteria swim only parallel or antiparallel with the magnetic field. The process is reversible, and alignment vanishes when the magnetic field is turned off.

At higher bacterial concentrations the system exhibits active turbulence. We study the magnetic control of the active turbulence in thin (ca. 60 μm) liquid films of highly concentrated bacteria on a glass slide, one side of the film facing oxygen rich atmosphere to maintain motility. Application of horizontal magnetic field on the turbulent-like suspension leads to gradual transition of the turbulence into nematically aligned state (Fig. 1). The nematically aligned state exhibits minute undulations and transverse flows, first signs of the emerging hydrodynamic instability. Releasing the aligning torque allows direct visualization of the progression of the hydrodynamic instability to full active turbulence.

Our findings show that magnetic torque mediated by a magnetizable medium can be a powerful tool for controlling both single particle dynamics as well as collective states of active particles. Major advantages include that the approach does not require use of special microorganisms (such as magnetotactic bacteria) nor magnetic tagging of the active particles.

Keywords: bacterial turbulence, active turbulence, magnetic fluids, ferrofluids

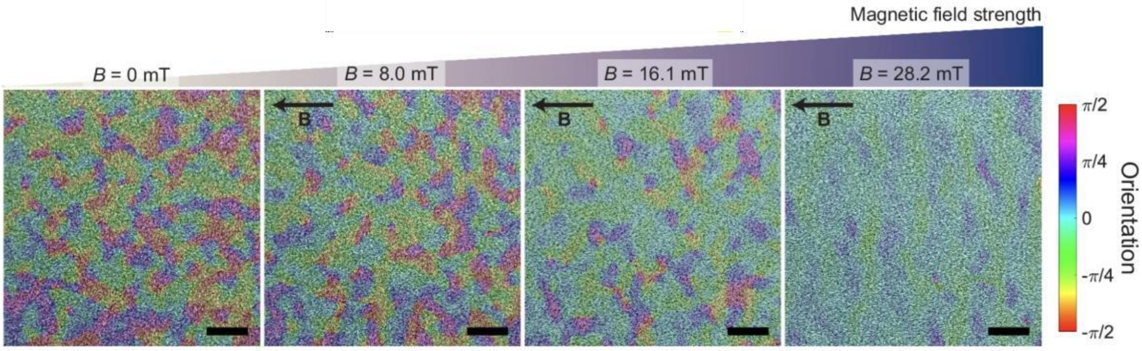

Figure 1. *Formation of undulated nematic order in a concentrated suspension of Bacillus subtilis bacteria in a magnetizable fluid upon increasing the strength of the external horizontal uniform magnetic field [1].*

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Odd elasticity in disordered chiral active materials

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Chiral active materials are composed of complex molecules that break both parity and time-reversal symmetry at the microscale. This is generally a result of continuous injection of energy and angular momentum through local torques, fueled by local energy consumption. These materials are abundant, from living matter such as the cytoskeleton twisted by motor proteins and self-spinning starfish embryos, to synthesized materials such as a fluid of rotating magnetic active colloids. The broken mirror-image symmetry, allows for the possible appearance of new type of elasticity dubbed `odd' elasticity [1]. This odd elasticity couples in a nonreciprocal way shear strains with shear stresses, and has been shown to give rise to remarkable mechanics. Current research of odd elasticity focuses on ordered structures, e.g., lattice designs of metamaterials. It remains less explored how odd elasticity can emerge in disordered elastic materials, which are ubiquitous in biological and synthetic systems. In this talk I will present a minimal generic Hamiltonian model for disordered chiral active materials, in which odd elasticity will naturally emerge in the presence of local active torques [2]. We use a two-dimensional continuum model of non-linear Cosserat elasticity, driven locally by active torques. We further study the viscoelasticity of such chiral active material immersed in chiral active fluid [3] and discover new type of propagating waves and new unreported instability regions in the dynamic phase diagram.

Keywords: chiral active matter, odd viscoelasticity, amorphous

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How Fluctuations Shape Collective Motion: Diffusive vs. Tumbling Dynamics of Flocks

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Collective motion is an example of an active matter phenomenon that breaks much of the intuition we might carry over from traditional soft matter physics, and as such it has been the focus of many studies over recent decades. It can be found across all length-scales in nature, from flocks of birds or crowds of people, all the way down to suspensions of bacteria. The most famous mathematical model for collective motion was proposed by Vicsek et al. in 1995 [1], with point particles that move at constant speed and try to align with their neighbours, but there is some error in this process due to random orientational fluctuations.

A common continuous-time variant is known as the "Flying-XY" model [2], which can be seen as consisting of Active Brownian Particles (ABPs) equipped with a Vicsek-style interaction. These ABPs are often used as a minimal model for bacteria; microscopic particles which self-propel through a thermal fluid in the over-damped regime, slowly changing direction diffusively over time. Many real bacteria, however, behave more like "Run-and-Tumble Particles" (RTPs) that "run" along straight trajectories while undergoing discrete "tumbling" events where they change direction. Despite this difference at the microscopic level, it was shown that in the context of "motility-induced phase separation" these two types of motion are equivalent [3], and it has typically been assumed to extend to the case of Vicsek interactions; the most common approach to coarse-graining the Vicsek model makes use of a tumbling-like approximation.

In our work we investigate whether this equivalence can be made, with initial indications being that while the overall structure of the phase-diagram is the same, there is a fundamental difference in the types of patterns found near the transition to collective motion. This highlights the crucial, but counterintuitive role of fluctuations in active matter.

Keywords: Collective motion, Vicsek model, pattern formation

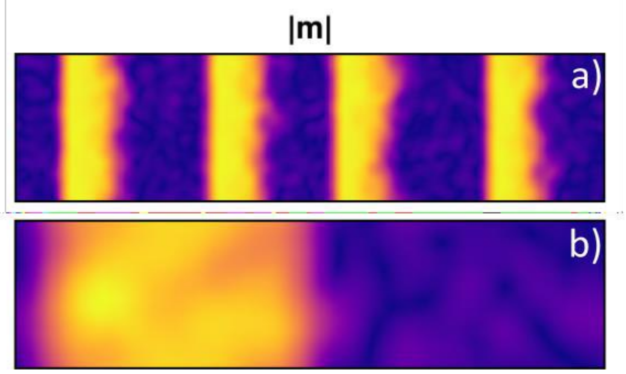

Figure 1. *Examples of the patterns found in the magnetization fields near the transition: a) ABPs, and b) RTPs.*

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Collective Motion and Hydrodynamic Instabilities in Surface-Confined Microswimmers

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The collective dynamics of swimming microorganisms is often dictated by long-ranged hydrodynamic interactions. One example is the collective motion of swimming, rear-actuated ("pusher") bacteria that interact through their long-ranged dipolar flow fields to create a state of so-called "bacterial turbulence" with chaotic, collective swimming with long-ranged correlations. This phenomenology contrasts with the behaviour of front-actuated ("puller") organisms such as certain algae, that do not exhibit any collective motion in unbounded bulk systems. For pushers, this state of collective motion is widely understood as a manifestation of a hydrodynamic instability due to the hydrodynamic alignment of pusher microswimmers. Unlike the idealised bulk setting, many experimental realisations of microswimmers instead involves swimming close to a solid surface or air-liquid interface, which effectively confines the swimmers' motion to a 2D plane. As I will show in this talk, this seemingly small restriction of the dynamics qualitatively changes the collective motion compared to bulk systems [1,2], due to previously overlooked physical effects. For pushers, the long-ranged hydrodynamic instability leading to bacterial turbulence in 3D is rendered short-ranged, with a collective state characterised by vortices of the order of the swimmer size. Additionally, we analytically and numerically demonstrate a previously unknown density instability of confined puller microswimmers, with no counterpart in unbounded systems. This instability occurs because the in-plane flow field of a single puller has a net-negative divergence even when swimming in an incompressible fluid, so that individual pullers on average act as hydrodynamic sinks. This leads to a dynamic attraction which induces a phase separation into dense puller clusters for high enough densities. Our results thus highlight that the experimental geometry can have a crucial impact on collective phenomena in active matter dominated by hydrodynamic interactions.

Keywords: Microswimmers, Collective motion, Hydrodynamic interactions, Bacterial turbulence

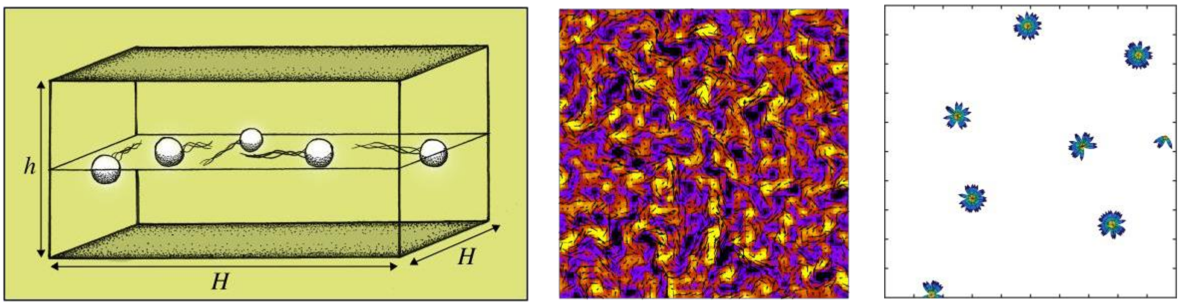

Figure 1. Left: *Schematic view of the simulated systems, with microswimmers confined to a 2-dimensional plane between two no-slip walls.* ***Centre:*** *Collective motion in a sheet of pushers, showing short-range fluid correlations.*
Right: *Aster-like clusters in a sheet of pullers. Reproduced from [2].*

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Novel active patterns emergent from nonreciprocal and transverse interactions

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Nonreciprocal forces violating Newton's third law are common in a plethora of nonequilibrium situations in soft matter science. While many recent studies have focused on two species with nonreciprocal coupling, much less is examined for the basic single-component system breaking the actio and reactio equality of force within the same species. We systematically derive the fundamental field theory of single-species nonreciprocal interactions from microscopic dynamics, leading to a generic framework termed *Active Model N* (*N* denoting nonreciprocity) [1]. We explore the rich dynamics of pattern formation in this intrinsic nonreciprocal system and the emergence of selftraveling states with persistent variation and flowing of active branched patterns. One particular new characteristic pattern is an interwoven self-knitting "yarn" structure with a unique feature of simultaneous development of micro- and bulk phase separations. For transverse interactions, we develop a phase-field-crystal theory appropriate for transversal interactions and find novel selfrotating odd elastic crystallites. Our predictions can be applied to various biological and artificial soft active matter systems controlled by single-species nonreciprocity or transverse interactions.

Keywords: non-reciprocal interactions, vision-cones, pattern formation, active field theory

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Active disordered elastic networks: Collapse, swimming, and subdiffusion with application to chromatin dynamics

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Motivated by the well-known fractal packing of chromatin, we study the Rouse-type dynamics of elastic fractal networks with embedded, stochastically driven, active force monopoles and force dipoles that are temporally correlated [1]. We compute, analytically – using a general theoretical framework – and via Langevin dynamics simulations, the mean square displacement (MSD) of a network bead. Following a short-time superdiffusive behavior, force monopoles yield anomalous subdiffusion, MSD $\sim t$, with an exponent identical to that of the thermal system, $\nu = 1 - d/2$, where d is the spectral dimension. In contrast, force dipoles do not induce subdiffusion, and the early superdiffusive MSD crosses over to a relatively small, system-size-independent saturation value. In addition, we find that force dipoles may lead to "crawling" rotational motion of the whole network and to network collapse beyond a critical force strength. We apply our results to the motion of chromosomal loci in bacteria and yeast cells' chromatin, where anomalous sub-diffusion with $\nu \simeq 0.4$ was found in both normal and ATP-depleted cells. We show that the combination of thermal, monopolar, and dipolar forces in chromatin is typically dominated by the active monopolar and thermal forces, explaining this observation.

We extend our studies to Zimm-type dynamics [2], with excluded-volume interaction included. The thermal and force-monopoles subdiffusion exponents are altered, yet the absence of subdiffusion for force dipoles is maintained. Moreover, force-dipoles produce translational center-of-mass diffusion (i.e. random swimming), in addition to the rotational crawling motion. We also discuss results from disordered fractals, both critical percolation clusters and clusters that are away from criticality, showing the effect of the isostatic point (known also as "rigidity percolation") [3]. We conclude by structure and dynamic studies of a collapsed chain model with added crosslinks as a specific model for chromatin and show that various broken exponents found for chromatin are theoretically recovered [4].

Keywords: Active system, fractal elastic networks, force monopoles, force dipoles, subdiffusion, micro-swimmers

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Active Brownian dynamics in a configurable viscoelastic media

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Active particles, both natural and artificial, when in complex fluid, show rich dynamical features such as anomalous diffusion and non-Boltzmann like behavior due to the interplay between the viscoelastic response of fluid, thermal fluctuations, and directed motion of the particle. When these microswimmers navigate through viscoelastic media, either the mechanism of inducing activity or the response of a microswimmer affects the local viscoelasticity of the medium, complicating the study of their dynamics. Hence, we asked whether a general experimental framework is achievable for investigating the dynamics of an artificial microswimmer in a fully programmable viscoelastic fluid. Here, we set up a programmable viscoelastic fluid by a diffusing optical trap to study the dynamics of a *phoretically active* Pt-coated polystyrene Janus colloid, where all the viscoelastic parameters can be tuned by changing the power of the optical trap and its diffusivity. To achieve this, a piezo-mirror is programmed to scan the optical trap following a computer-generated Brownian trajectory with the desired post-relaxation diffusivity of the active particle. The resultant response of the system behaves like a Maxwell-Voigt fluid that represents many viscoelastic soft materials, such as worm-like micelles, emulsions, and various linear viscoelastic materials. We also performed numerical simulations by modeling the system as *a harmonically bound active Brownian particle with long time diffusion*. The active particle exhibits Brownian diffusion at short time, intermediate anomalous diffusion governed by the competition between two timescales, i.e., the equilibration time and the persistence time, and long-time diffusion after the relaxation time. Finally, we discuss the possible ways to extract viscoelastic properties of the medium, such as the creep compliance, from the dynamics of the active Brownian particle, providing a framework for active microrheology.

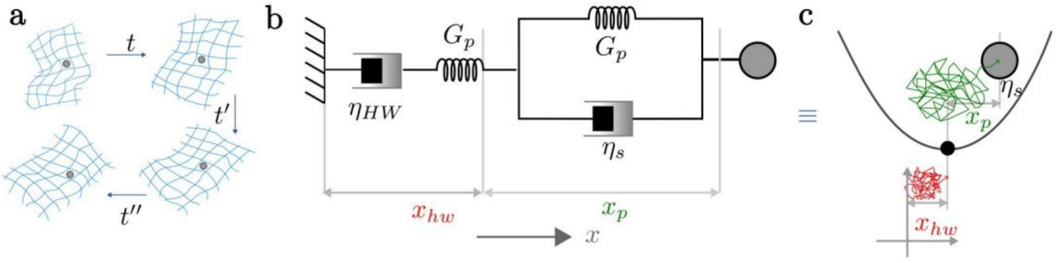

Figure 1: Graphical representation of (a) Active particle in a viscoelastic fluid, where internal polymeric structure changes over a timescale greater than the relaxation time. (b) The series combination of the Maxwell and Voigt models, which have matching elastic modulus G_p. η_{HW} and η_s represent the viscous dashpot for the Maxwell and Voigt models, respectively. (c) The dynamics of active Brownian particle in Maxwell-Voigt fluid can be modeled by harmonically bound active Brownian particle with long-time diffusion.

Keywords: active motion, optical tweezers, viscoelatic fluid

Acknowledgements: The authors acknowledge SERB, Govt. of India and Param Sanganak computing facility at the Computer Center, IIT Kanpur.

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Encoding Persistent Random Walks in Self-Propelled Particles: Lévy, Run-and-Tumble, Self-avoiding, and Gaussian

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Artificial microswimmers or micron-sized self-propelled particles have emerged as minimal model systems with unique capabilities, including autonomous motion, self-organization, and adaptability to local stimuli. Despite their significance in addressing fundamental questions in active soft matter and mimicking the dynamic self-organization of microorganisms, most synthetic self-propelled particles remain constrained to a single mode of autonomous motion [1], namely active Brownian particles (ABPs).

In this work, we present a novel experimental strategy to encode various types of persistent random walks in ABPs, drawing inspiration from the sophisticated search mechanisms of seabirds during foraging, predators during hunting, and certain bacteria with adaptive motility. Our approach enables precise control over multiple modes of motion, including Lévy walks with tunable step- length distributions, run-and-tumble dynamics, self-avoiding random walks, Gaussian walks, and trajectories shaped by potential landscapes [2]. Furthermore, we demonstrate the ability to steer particles along well-defined paths, including intricate geometric structures such as nested polygons and Fibonacci spirals. This versatility is achieved through the interplay between propulsion direction, precisely controlled via an external magnetic field programmed with an Arduino, and propulsion strength, dynamically modulated by varying light intensity. Additionally, we showcase rapid, on-demand switching between different modes of propulsion, highlighting the adaptability and control inherent in our system.

We demonstrate that the initial propulsion direction of individual ABPs allows the encoded random walks to evolve independently, in contrast to purely magnetic-field-steered systems, where all particles follow a common trajectory. This inherent stochasticity makes our system fundamentally distinct and more biologically relevant, closely mirroring the natural motility patterns observed in microorganisms. Ultimately, our study opens new avenues to explore how distinct types of random walks, encoded at the level of individual building blocks, influence dynamic self-organization and collective behavior in active matter systems.

Keywords: Levy walks, Encoding, Persistent random walks, Active Matter

Acknowledgments: We gratefully acknowledge the Netherlands Organization for Scientific Research (NWO) for funding through the NWO-M1 and XS grants.

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Isotropic-nematic transition of 3D active semiflexible filaments

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Active filaments are essential in biological systems, from motor-driven chromosomal DNA and actin filaments to worms. However, the impact of interplay between flexibility and activity on the isotropic-nematic (IN) transition remains largely unexplored. To address this, we conduct large-scale Brownian dynamics simulations of 3D semiflexible, tangentially driven active polymers [1]. In this regime, the IN transition of passive semiflexible filaments shifts to higher densities compared to their rigid counterparts due to anomalous nematic order fluctuations. These arise from collective deflections of worm-like chains twisted within an effective confinement tube, whose radius significantly exceeds that expected from solution concentration [2]. Actuating semiflexible polymers with tangential active forces further shifts the IN transition, the extent of which depends on degree of flexibility and activity level. Interestingly, the nature of IN transition changes from discontinuous at low activity to continuous for moderate activity levels. The shifted IN transition finds its origin in enhanced collective bending deformations resulting from energy injection at the particle scale, which increases the radius of the effective confinement tube. At moderate activity levels, enhanced collective excitations induce large-scale fluctuations, leading to dynamic steady states where the global nematic director evolves over time. Eventually, at sufficiently high activity levels, the IN transition is suppressed, giving rise to chaotic collective dynamics.

Keywords: Active matter, semiflexible active polymers, isotropic-nematic transition

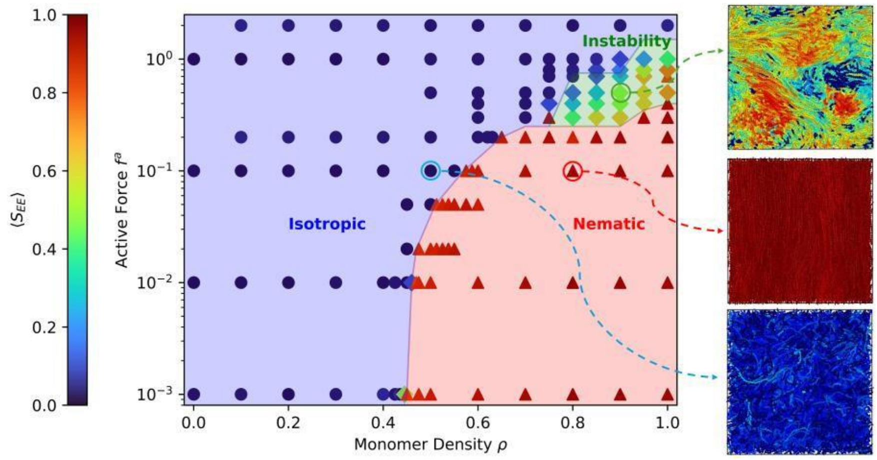

Figure 1: A state diagram of active semiflexible polymers as a function of monomer density and active force, in the three snapshots each polymer is colored with their local nematic order.

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Swimming on curved interface

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We study the dynamics of a colloidal microswimmer moving on a curved oil-water interface. To this end, we position a microswimmer onto the surface of a silicone oil droplet, 5 to 12 μm of radii, and analyse the dynamics of the microswimmer.

Unexpectedly, we observed that microswimmers present persistent propulsion in the horizontal plane around droplet's equator in addition to persistent propulsion occurring on the surface of the droplet. The persistent propulsion at the equator is observed over a range of tested droplet sizes and swimmer velocities, as well as viscosities of the oil. We compare our results with numerical simulations of self-propelled particles with persistence length, propelling on spheres. Finally, we propose additional experiments to elucidate the origin of this surprising effect.

Keywords: active particle, curved interface, persistent propulsion

Analyzing Active Nematic Dynamics: Transition from 3D to 2D Structures and Self-Assembly Processes

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Active matter refers to systems that consume energy from their surroundings, converting it into forces and motion, keeping them out of equilibrium and leading to diverse phenomena, from moving crowds to bacterial biofilms. This behaviour drives collective and stochastic dynamics, often linked to biological processes [1].

This study presents an active system with three components: an ATP reservoir, microtubules, and kinesin clusters walking along the microtubules. When brought to an oil-water interface, it forms a bidimensional active nematic material where "active turbulence" emerges due to its stochastic nature [2-3].

Previous studies have presented a methodology for in-situ photopolymerizing fixed 3D hydrogel structures, enabling observation of the photopolymerization process and active material response [4]. This approach has allowed for comprehensive studies of the material's rheology, including shear viscosity and activity parameter quantification, as well as quantitative mapping of forces around topological defects.

In this work, we present techniques to transition from fixed 3D structures to mobile 2D structures that are advected by active flows like rafts. This methodology allows us studying how the active fluid organizes and assembles these dispersed objects, providing insights into the spontaneous behaviour of active systems. The 2D structures also serve as a suitable cellular model, offering insights not only into how the material organizes obstacles, but also into how the active material behaves when laterally confined by 2D-like structures. This allows us to study the interaction between two active systems separated by an obstacle, which plays a crucial role in biological organization and may drive advancements in biohybrid machines.

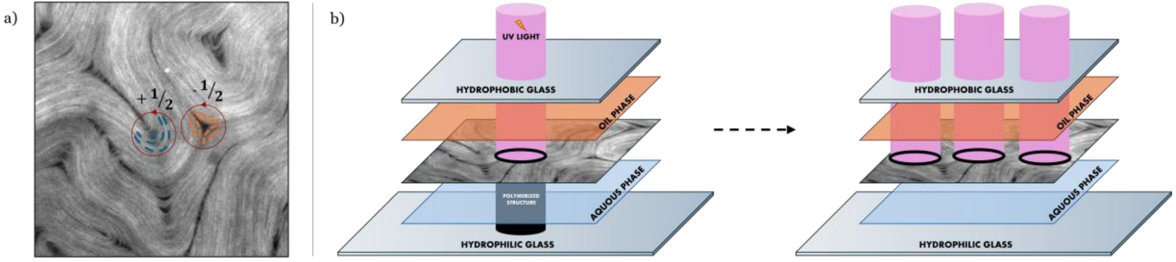

Figure 1. a) Bidimensional Active Nematic material depleted on an oil-water interface, +1/2 (blue) and -1/2 (orange) topological defects can be observed. b) Transition between the initial already studied 3D obstacles active system and the new one with 2D floating rafts.

Keywords: Active systems, Active nematic, Hydrogel, Photopolymerization, Self-assembly.

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Self-organization of FtsZ filaments drives enzyme transport in bacterial division

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Cell division requires the precise spatiotemporal coordination of numerous molecular machines. In bacteria, FtsZ filaments play a central role in recruiting and organizing the components necessary for division. These filaments assemble into highly aligned bands that encircle the cell, acting as a scaffold for division proteins. FtsZ filaments undergo treadmilling—growing at one end while shrinking at the other—which enables their self-organization into a well-defined ring [1].

Using coarse-grained molecular dynamics simulations, we model the dynamics of treadmilling FtsZ filaments and the enzymes that drive bacterial division. We find that combining the treadmilling dynamics of filaments within a ring and filament-enzyme attraction enables FtsZ filaments to transport enzyme particles toward the midcell, organizing them into a ring that is more sharply defined than the FtsZ filament ring itself. In particular, continuous formation and closing of gaps between adjacent strands of treadmilling filaments gives rise to a net particle flow toward the center of the FtsZ ring. We suggest that this mechanism allows FtsZ filaments to ensure that bacteria correctly divide at the midcell.

Our findings align with experimental observations showing that FtsZ treadmilling is required only in the initial phase of bacterial division [2]. Additionally, we demonstrate that FtsZ's ability to organize enzyme particles strongly depends on lateral crosslinking between neighboring filaments, consistent with previous experiments [3]. Overall, our simulations elucidate the role of treadmilling dynamics in bacterial division, highlighting how the self-assembly of FtsZ into a ring enables precise spatial control of wall-building enzymes during the early stages of cytokinesis.

Keywords: Cell division, FtsZ, Treadmilling, Active matter

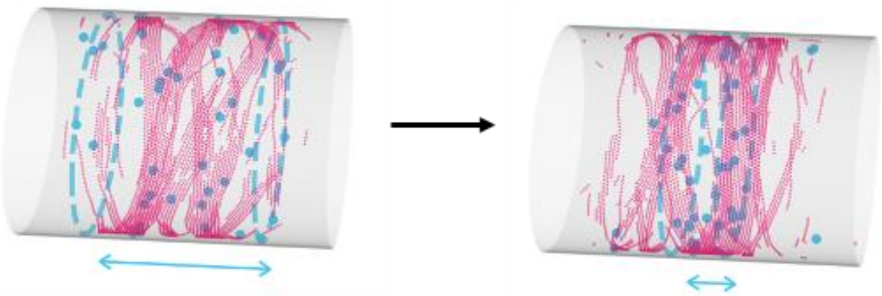

Figure 1. *Treadmilling filaments (pink) transport enzyme particles (blue) towards the midcell.*

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Designing responsive inks for multi-material reconfigurable microrobots via 2PP

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Two-photon polymerization (2PP) enables high-resolution additive manufacturing of microscale structures, revolutionizing fields such as soft robotics, microfluidics, and biomedical engineering. However, integrating responsive materials into complex, spatially programmable microstructures remains challenging, often limited by single stimulus-responsives or planar geometries. Previously, we introduced a method termed 'Printing on Particles' (PoP) to fabricate multi-material microstructures. [1] This approach combines two-photon polymerization direct laser writing (2PPDLW) with sequential Capillary Assisted Particle Assembly (sCAPA), enabling precise placement of microparticles and constructing complex mutli-material structures. In this study, we extend the range of printable materials via PoP to include soft, shape-reconfigurable materials that can serve as active, responsive components in microrobotics systems. By utilizing three distinct thermoresponsive monomers (NNPAM, NIPAM, and NEAM) and blending them in various ratios, we developed inks with tunable volume phase transition temperatures (VPTT) ranging from 20°C to 60°C. Furthermore, we enhance the selectivity of these soft inks by incorporating nanoparticles with different plasmonic absorption peaks. Specifically, we successfully integrated gold nanoparticles (AuNPs), silver nanoparticles (AgNPs), and gold nanorods into a single printed hydrogel-based (pNIPAM) microstructure, which shows spectrally-resolved actuation. The ability to incorporate functional nanoparticles constitutes a versatile platform for the development of a new class of fully autonomous active materials.

Keywords: Active Matter, Micro-fabrication, Two Photon Lithography

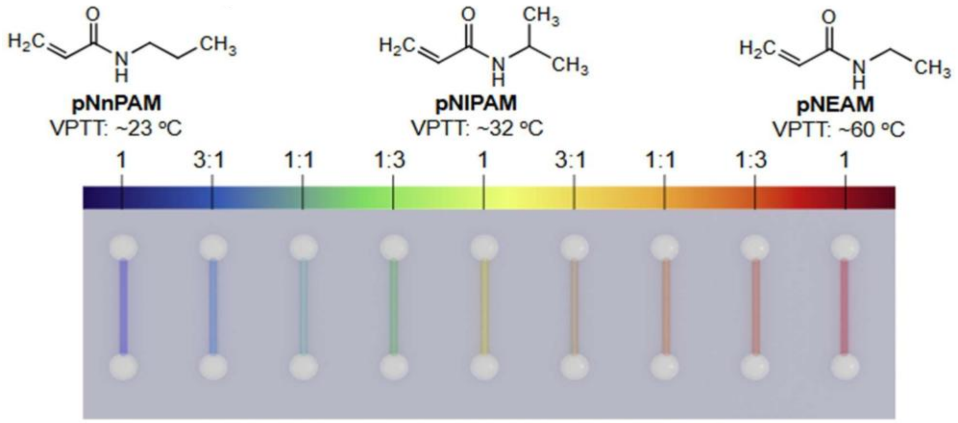

Figure 1. Schematic of various 2PP fabricated thermo-responsive links with tunable VPPT connecting silica beads

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Swirling and Directed Swarm Assembly due to Misaligned Perception-Dependent Motility

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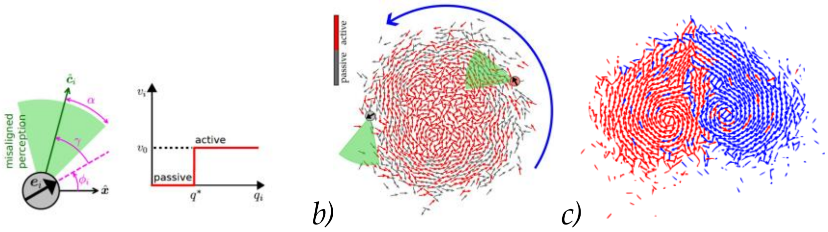
Self-assembly into cohesive, swirling or swarming groups is a frequent strategy used by living organisms in a wide range of length scales, and an inspiration for the design of synthetic active smart materials. Navigation strategies based on a visual-type of perception are intrinsic to many living systems and result in a very rich variety of flocking behaviors, such as aggregation, milling, or meandering. Visual-type of perception restricts the interactions to neighbors placed inside a finite cone with propulsion direction as the symmetry axis and tip at the particle position. A computer assisted feedback loop to control the individual interactions of synthetic colloids has shown to form cohesive groups for systems with particle interactions varying their motility in terms of visual-type of surrounding perception [1]. Here a system of particles with motility variable in terms of a visiontype of misaligned perception-dependent motility is investigated by a combination of Langevin dynamics simulations in two-dimensional systems together with an analytical approach based on conservation law principles [2]. Persistent swirling with predetermined direction is induced by the misalignment, this is by differentiating the self-propulsion direction and the perception cone axis, see Fig.1a. Clusters can have a fluidlike center with a rotating outer layer or display a solid-like rotation driven by the outer layer activity, see Fig.1b.

A mixture of particles with perception-dependent motility and opposite misaligned visual perception shows to spontaneously self-organize into a self-propelling bean-shaped cluster [3]. The two species initially rotate in opposite directions, which together with the steric interactions, makes them segregate into two main counter-rotating domains forming a cohesive and persistently propelling single cluster, see Fig.1c. Discontinuous motility with misaligned perception might therefore serve as a powerful self-organization strategy in microrobots and a promising pathway for the design of programmable active matter.

Keywords: Swarm intelligence, Active matter, Self-assembly, Janus colloids



a) *b)* *c)*

Figure 1. a) *Illustration of an active particle with misaligned visual perception, where the vision cone is oriented differently than the propulsion, and the particles become active when perceiving enough neighbors. b) Snapshot of a swirling cohesive cluster. c) Snapshot of self-assembled swarming cluster composed of a mixture of particles with left and right misaligned perception.*

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Monday 29th September 2025

I.Interfaces, surfaces, membranes, emulsions

(Room 2)

Chemically active interfaces: a route to enhance and control catalysis

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In many circumstances spanning from catalysis in industrial reactors to biological scenarios, chemical reactions occur within thin liquid films. While for thin film in non-reactive conditions the key physical process determining their stability have been identified since long, this is not the case for thin film hosting chemical reactions. In fact, the inhomogeneity in the density of both reactants and products induced by the chemical reaction may alter the non-reactive picture.

By means of simple semi-analytical models, I will discuss how this can occur in two main scenarios.

First, in the case of plane thin films, I will show that the inhomogeneous densities of reactants and products will lead to Marangoni flows, which not only affect the stability of thin films but can also induce novel dynamical regimes, such as travelling and standing waves, absent in the passive counterparts. I will critically discuss these results, and I will emphasize the experimentally relevant scenarios where these phenomena can be observed [1].

Next, I will discuss the problem of chemical reactions within droplets. For this case, I will show that the ~100-1000 fold enhancement in the rates of chemical reactions observed experimentally [2] is indeed not due to an enhancement of the effective reaction rate, but rather by the local change in chemical potential due to the effective interactions between the chemical compounds and the interface. I will critically discuss these predictions by showing recent experimental data which qualitatively confirm them [3].

Keywords: thin film, Marangoni flow, catalysis

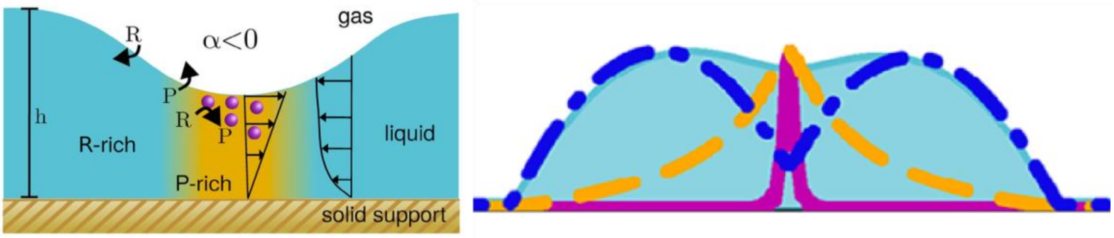

Figure 1. *Left: cartoon of a thin liquid film containing particles (violet) which catalyze chemical reactions. Right:*
droplet shape (light blue), particle density (violet), reactant density (dot-dashed blue), and product density (dashed orange) for a droplet under reactive conditions.

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P. Malgaretti, T. Nizkaya, J. Harting, in preparation

Influence of Domain Size and Topology on the Shear-induced Sponge-to-Lamellar Transition in Bicontinuous Microemulsions

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Understanding and engineering the flow-response of complex fluids formed by surfactant membranes is a key challenge for their practical utilization. Nevertheless, the predicted sponge-to-lamellar transition of self-assembled surfactant membranes upon shear flow [1] has, to our knowledge, only been shown for surfactant bilayers [2]. Via the combination of small-angle neutron scattering and microfluidics [3], we recently investigated the influence of shear flow on the sponge-like surfactant monolayer of a model D_2O/*n*-octane/$C_{10}E_4$ bicontinuous microemulsion and demonstrated for the first time its gradual transition into a lamellar-like structure [4]. Extending our study, we exposed different bicontinuous microemulsions to microflows of up to 40 mL min^{-1}, resulting in shear rates above 10^5 s^{-1}. Quantitative analysis of the recorded scattering data shows that the domain size of the original bicontinuous structure, given by the volume fraction of the surfactant membrane, dominates its response to shear for more diluted samples. While their shear-induced structural changes simply scale with the membrane volume fraction, the stronger response of higher concentrated microemulsions near the bicontinuous/lamellar coexistence points to the influence of an altered topology [5]. Furthermore, one can even amplify this response by doping the surfactant monolayer with amphiphilic diblock copolymers [6]. Known for their efficiency boosting effects [7], these polymers modify the elastic properties of the surfactant membrane and therefore also the topology of the initial bicontinuous structure [8]. Finally, using a phenomenological approach, we are able to generalize the topological influence and provide a uniform description for the shear-induced transition of a bicontinuous microemulsion into lamellae [6].

Keywords: bicontinuous microemulsions, microfluidics, SANS, sponge-to-lamellar transition.

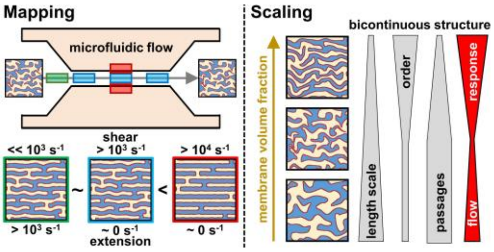

Figure 1. *Small-angle neutron scattering studies inside a microfluidic constriction reveal the gradual transition of bicontinuous microemulsion under shear, forming a lamellar-like structure facilitated by the disintegration of remaining passages (taken from [5]).*

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Curvature-dependent adsorption of surfactants in water nanodroplets and nanobubbles

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Surfactants, molecules that readily adsorb to liquid interfaces and reduce surface tension, have been a focus of scientific research for nearly a century. Nevertheless, while their behavior on flat surfaces is well-studied, their interactions with tiny, curved surfaces, such as those in nano-sized droplets and bubbles, have remained elusive and largely unexplored, primarily due to challenges in direct experimental observation. To shed light on this aspect, we perform molecular dynamics simulations of short-chain surfactants in nanodroplets and nanobubbles (see figure), and investigate how curvature impacts the adsorption at the water- vapor interfaces.

The outcomes reveal that adsorption systematically depends on curvature, being enhanced on droplets and reduced on bubbles, with the effect becoming more pronounced for surfactants with longer hydrophobic tails. We attribute this curvature-dependent behavior to two key mechanisms: Laplace pressure and curvature-dependent surface tension. The breakdown of these contributions allows us to develop a simple theoretical model that offers a quantitative view of these mechanisms and is able to predict the influence of curvature on adsorption, particularly for longer-chain surfactants.

We investigate this phenomenon also in droplets deposited on a substrate, where the effect of curvature remains relevant, but surfactants can be adsorbed also at the water- substrate or at the vapor-substrate interfaces. This has an effect on their shape [1], displaying a strong size-dependent behavior [2].

These results have broad implications across various fields, from cloud formation and climate modeling to the stability and reactivity of nanodroplets and nanobubbles.

Keywords: Surfactants, Adsorption, Molecular dynamics simulation

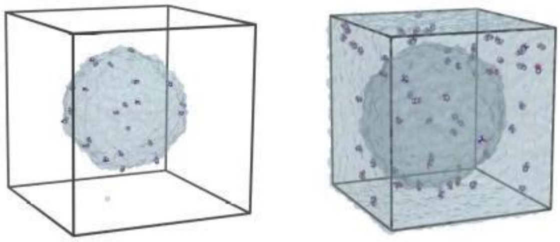

Figure 1. *Simulation snapshots of a droplet (left) and a bubble (right). Surfactants (in this case propanol) are shown in all-atom representation while water is represented as a transparent smoothed density isosurface.*

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The stability of natural marine foams

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The appearance of marine foam on coastlines can be observed all over the world. In particular, a remarkably stable and abundant foam is observed annually along the Opal Coast from April to June, often persisting for several days and reaching heights of up to one meter (see Fig. 1a). The formation of this foam is consistently correlated with the accumulation of a microalga called *Phaeocystis globosa* in seawater ("a bloom") [1,2].

We aim to understand the reason for the ultra-stability of marine foams. In this presentation, we specifically study the role of algal proteins in the generation of this natural marine foam.

A series of field samplings was carried out in the spring of 2023. Marine foam was collected, and its liquid (see Fig. 1b) was stored for further analysis.

Back in the laboratory, we developed a method to identify and quantify the amphiphilic materials responsible for foam stabilization, based on knowledge of the physicochemical properties of foams [3,4]. We "refoamed" the liquid using a controlled bubbling process and measured protein depletion in the liquid during foam generation. The results of this study suggest that algal proteins play a major role in foam stabilization.

However, the marine foams are ultrastable, a property that requires the presence of a co-component in addition to the amphiphilic component (here, the proteins). I will present the possible role of two co-ingredients that could enhance the stability of marine foams: polysaccharides and sediment aggregates present in our samples.

Keywords: Marine Foam, Foam Stability, Algal proteins

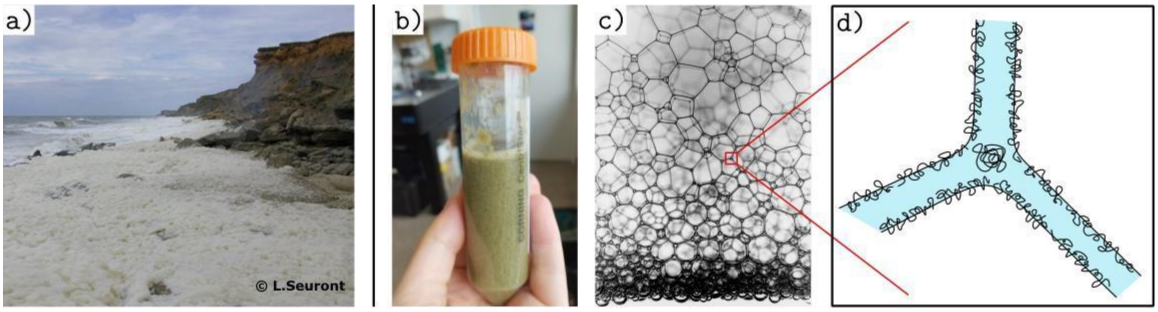

Figure 1. *a) a foaming event; b) field samples; c) foam structure; d) proteins at the interfaces.*

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Tuning Pore Size in Integral-Asymmetric, Isoporous Membranes via Bidisperse Diblock Copolymers

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Integral-asymmetric isoporous membranes, widely used in water filtration, are fabricated using a combination of evaporation-induced self-assembly (EISA) and nonsolvent-induced phase separation (NIPS), collectively termed SNIPS. This method enables a two-step, bottom-up process to produce an isoporous top layer for efficient filtration, supported by a mechanically robust substructure. For practical applications, membranes must have pores of an optimal size—small enough to selectively block target substances but not so small as to cause excessive water resistance. Developing techniques to achieve tunable pore sizes could broaden their utility across diverse applications.

While pore size can technically be adjusted by varying the copolymer's degree of polymerization, this approach requires synthesizing new copolymers for each desired pore size, leading to high costs. A more economical alternative is blending polymers, where tuning the blending ratio of different components offers a feasible way to control pore size. In this study, we employ self-consistent field theory and particle-based simulations to explore the ordering dynamics of bidisperse diblock copolymers via both rapid quenching and solvent evaporation. Specifically, we will focus on (1) examining the dependence of the equilibrium cylinder/pore size on the blend composition, (2) understanding how the parameter region of macrophase separation is suppressed during the ordering process, leading to an enlarged effective blending window, and (3) elucidating how the ordering dynamics affect the final cylindrical/porous structure. Our findings provide valuable insights for the cost-effective fabrication of filtration membranes with tailored pore sizes.

Keywords: block copolymers, isoporous membrane, solvent evaporation, phase separation, SNIPS

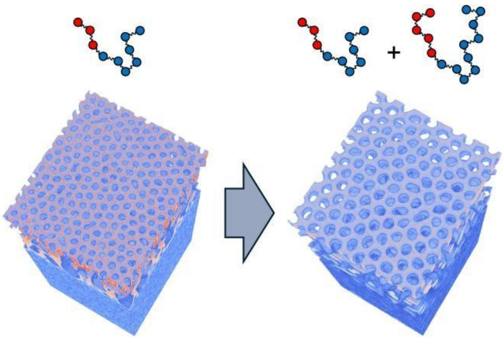

Figure 1. *Comparison between the porous structures produced by SNIPS using monodisperse (left) and bidisperse (right) diblock copolymers.*

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Engulfment of microgels by membrane wrapping

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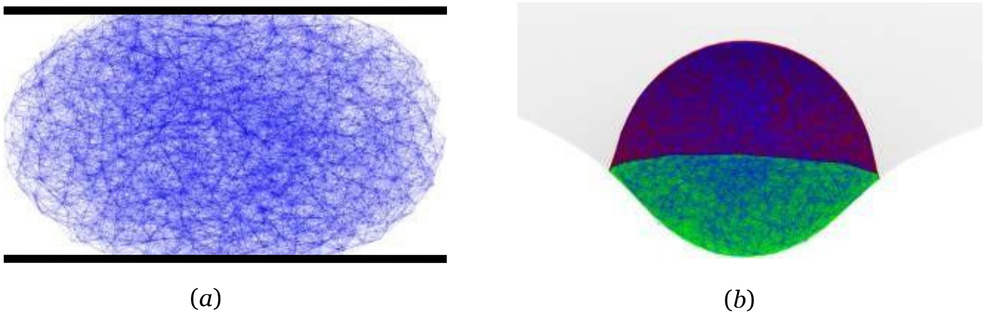
The interaction of nano- and microparticles with lipid membranes plays a key role for cellular engulfment of cargo [1]. Microgels with tunable size, shape and deformability are a versatile system for understanding the interaction of elastic particles with membranes [2]. Using a spring network model for the microgels and triangulated surfaces for the membranes, we study microgel wrapping at lipid-bilayers. First, we simulate microgels confined between two parallel walls to characterize their Young's moduli and Poisson's ratios. We then determine the interplay of microgel and membrane deformation controlled by the competition between membrane bending rigidity and microgel elasticity. Our calculations predict an increased stability of partial-wrapped states for microgels with lower Young's moduli [3]. There is a discontinuous transition from oblate microgel shapes at low wrapping fractions to cup-like shapes at high wrapping fractions. At membranes with high tension, we also observe another discontinuous transition at deep-wrapped states between cuplike shapes of microgels and nearly spherical shapes [3]. Our results will allow the design of the microgels with optimal elastic properties for biomedical applications, such as targeted drug delivery.

Keywords: membranes, microgels, elasticity, bending rigidity, wrapping



(*a*) (*b*)

Figure 1. *An initially spherical microgel (a) in-between two parallel walls and (b) attached to a membrane.*

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Interfacial Stresses in Foams: From Microscale Film Dynamics to Macroscale Stability

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The stability and rheology of multiphase materials, such as foams, are largely governed by the properties of their interfaces and the behavior of thin liquid films (TLFs) separating interacting droplets or bubbles. When two bubbles come into close proximity, a TLF forms between them and progressively thins through drainage. This thinning process, along with the overall stability of TLFs, is strongly influenced by interfacial stresses and intermolecular interactions driven by surface-active species.

In this talk, we will discuss how experimental techniques, such as the dynamic thin film balance and interfacial shear rheometry, shed light on nano- and micro-scale physics of these materials. Particular attention will be given to films stabilized by low molecular weight surfactants, copolymers, and plant proteins, and how they impact key foam destabilization processes: drainage, coalescence, and Ostwald ripening. We will show that foam half-life is directly related to the type and magnitude of interfacial stresses, as well as to the thickness of the TLFs that separate two bubbles. A universal picture on foam stability emerges, which enables the rational design of sustainable foams.

Keywords: thin liquid films, foams, surfactants

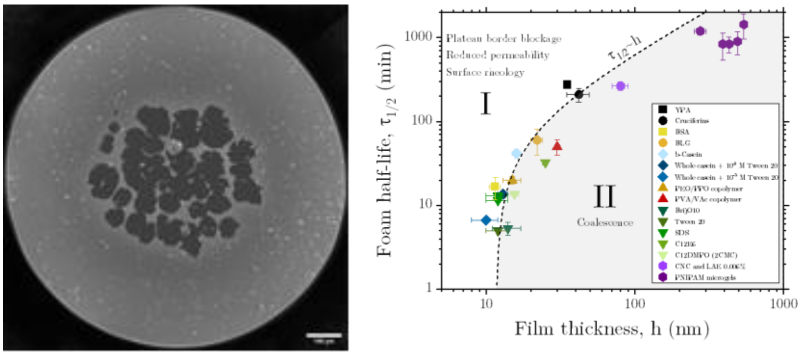

Figure 1. *: (Left) Microinterferometry image of a foam film stabilized by a protein (yellow-pea albumin). (Right) Correlating foam half-life with film thickness.*

Acknowledgements: The author acknowledges the contributions of Jan Vermant (ETH Zurich), Jack Yang, Costas Nikiforidis, and Leonard Sagis (Wageningen University) in parts of this work.

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Softening Effect of pNIPAM Microgels on Pickering Emulsions: Drop Deformation and Elasticity

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Pickering emulsions are surfactant-free, metastable dispersions of two non-miscible fluids stabilized by the adsorption of particles at the interface. Particle characteristics, including softness, deformability, and particle-particle interactions, primarily determine the stability. Many applications necessitate their destruction upon use. Thermo-responsive microgels swell at room temperature and shrink when heated beyond their volume phase transition temperature (VPTT). The most commonly used microgels are made of poly(N-isopropylacrylamide) (pNIPAM) and exhibit a volume reduction at 33 °C [1]. Typically, microgels synthesized through the precipitation polymerisation of pNIPAM exhibit a more crosslinked core enveloped by a fuzzy shell of dangling polymer chains. Consequently, microgels adopt a "fried-egg" structure when adsorbed at interfaces. The core undergoes slight deformation while the dangling chains extend, forming a thin, flat corona around the core. In this work, we explore thermoresponsive oil/water emulsions stabilized by various microgels of differing softness ($R_h \sim 150$ nm): Ultra-Low Crosslinked (ULC) microgel, regularly BIS-crosslinked microgels (1 mol% and 2.5 mol% N,N′-methylenebis-acrylamide (BIS)), and linear pNIPAM. We found that oil droplets stabilized by the microgels can deform in crowded environments and depend on the polymer concentration and the softness. This droplet deformation is more pronounced when ULC microgels stabilize the oil droplets, demonstrating a significant effect on the dispersed phase due to these microgels' compressibility and deformability characteristics. To understand the impact of the microgels on the deformed oil droplets, we investigated the interfacial viscoelasticity of the droplets in terms of the interfacial dilational moduli of oil drop. Additionally, we linked these findings to the interfacial viscoelasticity properties using a rheometer equipped with a custom-made double wall-ring accessory and a purpose-built Langmuir trough [2].

Keywords: Pickering emulsions, pNIPAM microgels, softness, droplet elasticity.

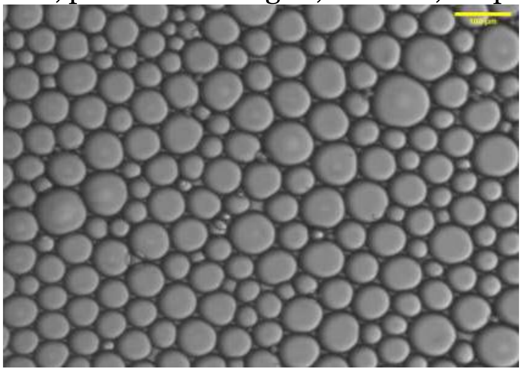

Figure 1. Deformed oil droplets stabilized by ULC microgels in a crowded environment (0.25 wt % of microgel). The scale bar is 100 µm.

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Silicone Nanofilament Coated Membranes for Membrane Distillation

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Globally, water shortage has emerged as a major issue. To create more usable water, membrane distillation (MD) has gained relevance as a desalination technology [1]. The main disadvantages of current membranes for membrane distillation are their low wetting resistance, relatively low vapor permeation flux and the fact that they contain fluorine. Silicone nanofilaments (NF) coated membranes appear as an interesting alternative to be applied on this field. The coating provides superhydrophobicity to the porous membrane. At the same time, the obtained coated membranes exhibit large vapor permeation flux [2].

The coating comprises the plasma activation of the substrate membrane for obtaining –OH groups, followed by hydrolysis and condensation of trichloromethylsilane (TCMS). Usually, this procedure is conducted overnight in organic solvent. Fabrication of fluorine-free superhydrophobic membranes using a non-aromatic solvent was accomplished. Polypropylene (PP) and polyethersulfone (PES) porous membranes were tested as substrates for the coating. NF coating grows on hydrophilic substrates like PES, while scarce filament growth was observed on PP membranes. Coated PES membranes were tested in membrane distillation with permeation fluxes in the same order than standard PTFE membranes and salt rejection close to 100%, when using a synthetic seawater sample as feed. Despite the low acid resistance of the membranes, they exhibit better antiscaling and antibiofouling properties than standard PTFE samples [3].

Keywords: Membrane distillation, superhydrophobicity, scaling, biofouling, silicone nanofilaments.

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Light-responsive coacervates for synthetic protocells

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Liquid-liquid phase separation (LLPS) is a fundamental mechanism for assembling biomolecular condensates in living cells and offers a powerful strategy for creating dynamic synthetic compartments with life-like properties. Coacervation between oppositely charged species has been widely used to model these membraneless compartments [1], yet achieving controlled dynamics over coacervation remains challenging. To introduce external control over LLPS, we developed photoswitchable DNA-azobenzene coacervates, where light triggers reversible droplet assembly and dissolution (Figure 1A) [2]. These systems laid the foundation for engineering synthetic condensates with tunable dynamics, enabling precise, light-actuated biomolecule storage and release.

Expanding on this approach, I will discuss the design of minimal light-responsive coacervates using azobenzenes of variable charge valency and mononucleotides [3]. We show that the charge valency of both azobenzene and nucleotide components plays a crucial role in governing coacervation behavior. Additionally, we observe a clear preference for purine-based nucleotides over pyrimidines, underscoring the impact of nucleotide chemical structure on phase behavior. The reversible *cis-trans* azobenzene photoisomerization offers a robust strategy for modulating phase separation in these minimalistic droplets, allowing precise control over coacervate properties in response to light. We further demonstrate light-actuated hierarchical droplet organization and biomolecular localization within multiphase coacervates (Figure 1B).

Taking this concept further, I will briefly exemplify how photoswitchable coacervation can be leveraged to regulate non-enzymatic reactions [4]. Using end-reactive oligonucleotides, we are able to control on/off polymerization through cycles of light-induced phase transitions. Notably, polymerization influences polynucleotide length distributions, driving phase transitions that result in multiphase coacervates via length-based DNA self-sorting (Figure 1C).

Overall, our work establishes light-actuated coacervates as a versatile platform for studying energy-driven phase separation. By integrating tunable droplet dynamics with reaction control, we provide a minimal model for protocellular organization.

Keywords: coacervates ● protocells ● azobenzenes ● DNA ● light-responsive systems

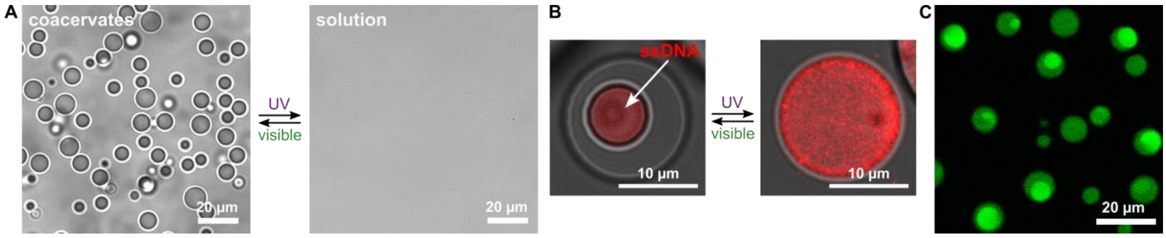

***Figure 1. A**, Light-responsive assembly/dissolution of coacervates. **B**, Controlling multiphase coacervates with light. **C**, Oligonculeotide polymerization-induced self-sorting*

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Bidirectional crystal growth and intermittent dynamics during confined evaporation of salty solutions

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Salt creeping, a process where crystals precipitate far away from the interface of an evaporating salt solution, is a well-known phenomenon with broad implications in inkjet printing and outdoor electronics. Herein, we explore the dynamics of crystal growth during the confined evaporation of salty solutions from one end of a capillary (figure 1a). As the solvent (water) evaporates from the lower end of the capillary, we observe that the salt crystals start depositing on the outer surface of the capillary. A careful investigation on the growth of salt crystals reveals two distinct directional modes: axial growth—where crystals grow axially on the outer surface of the capillary, and radial growth—where they grow laterally along the rim. Through a systematic variation of the initial salt concentration and relative humidity, we explore the influence of these factors on the directionality of salt growth. Moreover, the speed of the evaporation front exhibits non-monotonic temporal dynamics during salt creeping (figure 1b). We construct a simple analytical model, which elucidates how the hysteresis associated with hygroscopic growth of salty solutions results in the intermittent temporal dynamics (figure 1c). The findings of this study deepen our understanding of salt creeping in confined geometries, and the underlying physics of bidirectional crystal growth and intermittent dynamics.

Keywords: evaporation, crystallization, hygroscopic growth, microscale transport

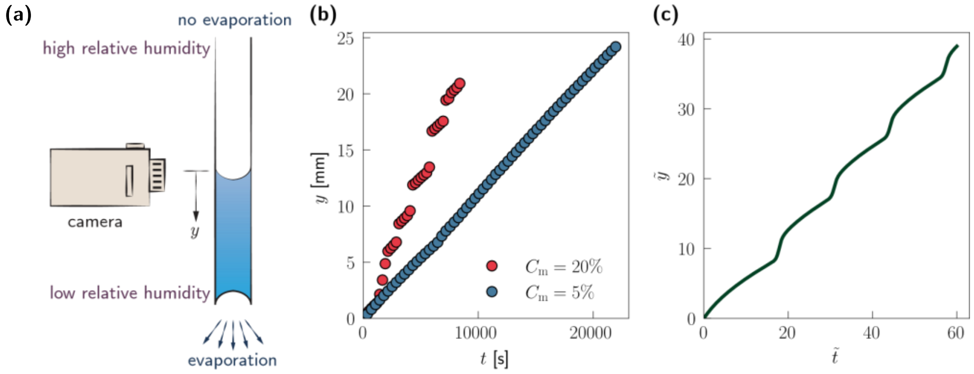

Figure 1. *(a) Schematic of the experimental setup. (b) Temporal variation of evaporation front can exhibit either monotonic or non-monotonic dynamics depending on the salt concentration (C*m*). (c) Analytical prediction of the normalized evaporation front location with normalized time also exhibits intermittent dynamics.*

Switchable Cavitation in Soft Matter

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Stimuli-responsive buckling, wrinkling and creasing on the surface of soft polymers and gels can be used for design of self-assembled materials and sensors and have been intensively studied in the literature [1]. Recently, similar phenomenon have been explored in non-flat geometries, for example on a surface of a spherical cavity within an elastic solid [2]. Moreover, a new phenomenon of reversible opening/closing of small spherical cavities was observed and has potential applications [3]. In a possible explanation, a soft pore (Figure 1. a) may be bistable (i.e., may remain an infinite amount of time in both closed and open state) due to the competition between the adhesion energy of inner surfaces of the cavities and the strain energy inside the matrix. However, the role of surface instability and of interfacial interactions remains poorly understood.

In this work, we performed finite element simulations and experimental investigation of compression of model soft pores. On the Fig 1.a, we show the total energy of a 2D pore in a neo-Hookean elastic matrix with an adhesive contact between the pore walls as a function of the normalized contact surface $A_{\text{closed}}/A_{\text{total}}$. By varying the ratio $\frac{E*R}{\gamma\text{PDMS}}$ where E is Young's Modulus, R is the initial radius of the pore, γ_{PDMS} is the surface energy of the matrix, we demonstrated the bistable behavior at intermediate values of R. When R is small, the E_{total} decreases with A_{closed} which means the pores will spontaneously collapse. For large pores, the release of the external force will lead to reopening of pores.

In experiments, isolated pores inside a soft PDMS matrix were fabricated via emulsion technique and the sample was compressed (Fig 1.b): we show that pores remain closed after the force is released which is due to the adhesive force.

Keywords: Instabilities, Elastomers, Mechanics.

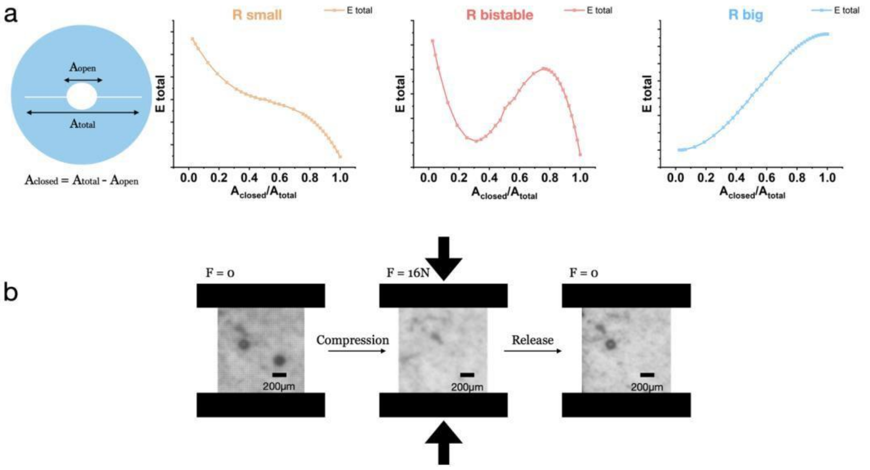

Figure 1. *(a) Total energy of the pores changing with the pore size. (b) Two pores inside the PDMS matrix closed by 16N compression but one pore remains closed after releasing the force.*

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Unraveling the Molecular Origins of Slippery Behavior in Tethered Liquid Layers

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Slippery covalently attached liquid surfaces (SCALS), such as polydimethylsiloxane (PDMS) layers, exhibit ultralow contact angle hysteresis (CAH), making them ideal for self-cleaning and antifouling applications. Recent studies identify a "Goldilocks zone" of optimal performance at intermediate PDMS thicknesses (~4 nm) [1], but the origins of this behavior and the variability in CAH across similar layers are not fully understood.

Combining coarse-grained molecular dynamics (CG-MD) simulations and atomic force microscopy (AFM) experiments, we reveal that nanoscale defects and layer deformation govern SCALS performance [2]. At low thicknesses, incomplete substrate coverage creates chemical patchiness, increasing CAH. At higher thicknesses, polydispersity-induced lateral microphase separation generates nanoscale waviness, while layer deformation at the droplet contact line further elevates CAH (Fig. 1). Surprisingly, these static wavy features arise from polymer chain segregation by length—a phenomenon not previously observed in liquid-like grafted polymers.

We find that optimal slippery behavior occurs in smooth, chemically uniform layers without significant waviness or deformation. Polydispersity, however, increases surface roughness and deformability, raising CAH. These insights highlight the complex interplay between chain length, grafting density, and thickness in SCALS performance, while offering design principles for surfaces with ultralow CAH and uncovering new phenomena in tethered liquid layers.

Keywords: Polymer brushes, PDMS, MD simulations, AFM mapping, Contact angle hysteresis

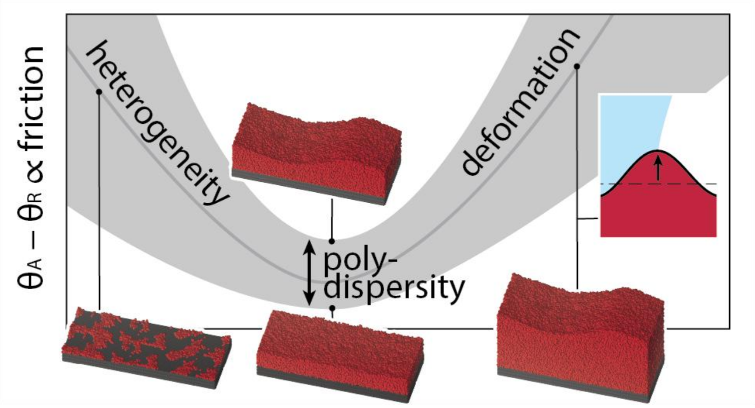

Figure 1. *Combined simulation and experimental study of SCALS explain the "Goldilocks zone" for slippery surfaces.*

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Unravelling the multiscale surface mechanics of soft solids

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The mechanics of soft solid interfaces is key to the response of many natural and artificial systems at small scales. Yet, their underlying properties are vigorously debated, particularly for polymer networks. While molecular-scale theory predicts no interfacial changes with macroscopic deformation, multiple experiments suggest that interfacial tension increases with strain. To settle this issue, we here focus on the measurement of displacement fields near the interface of a deformed silicone gel, in the limit of small deformations. We observe an unexpected multiscale response. The shear modulus drops by a factor of two smoothly over 20 μm near the interface. At the same time, we observe a surface excess elasticity, due to an unresolved gradient, that depends on the composition of the outer medium. Together, these results demonstrate that the mechanical response of soft polymeric solids is intrinsically multi-scale, and demand further experimental and theoretical investigations into soft solid interfaces.

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pH-Responsive Colloidal Gates for Tunable Liquid and Molecular Transport

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We present the design and development of pH-responsive colloidal systems with tailored interfacial properties to enable the controlled transport of liquids and molecules. Inspired by the natural swelling and shrinking behavior of clay particles in response to changes in pH, we have engineered sub-micron silica colloids with densely grafted pH-sensitive polyelectrolyte brushes.These ”colloidal gates” exhibit reversible volume transitions upon variation of the solution pH, effectively modulating the transport of liquids and molecules through a fixed-bed column packed with the particles [1]. At higher pH values, the polyelectrolyte brushes undergo deprotonation, leading to particle dispersion and increased permeability of the column. Conversely, at lower pH, the protonated brushes promote particle coagulation and reduced transport. By systematically investigating the coagulation and dispersion behaviors of the pH-responsive particles as a function of ionic strength and pH, we have correlated these interfacial properties with the observed transport phenomena. Our results demonstrate the key role of surface forces and interparticle interactions in governing the permeability of the colloidal system [2]. This work showcases the potential of stimuli-responsive colloidal gates as a versatile platform for the development of smart separation and filtration technologies, with applications ranging from water purification to drug delivery.

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Heterogeneous decoration of ionic mesopores by ionic and poly(ionic) liquids

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Understanding the molecular structure of mesoporous solid ionic systems is crucial for optimizing macroscopic properties, in particular ionic transport for energy applications, as well as mechanical flexibility. These systems can be synthesized efficiently under "one-pot" conditions, which rely on mesopore formation through microphase separation of templating ionic liquids [1].

In the present study, poly(ionic liquid)s have been added in order to incorporate both connectivity and modify mechanical strength [2]. We report on the structural analysis of ionic liquid and poly(ionic liquid) embedded in ionosilica matrices, employing a combination of small-angle scattering of neutrons and X-rays, isotopic substitution, and physico-chemical solvent-based extraction methods. Data analysis is based on molecular modelling with an original, quantitative comparison of the scattering curves under different contrasts. In agreement with NMR, it is shown that these mesoporous systems have an unexpected molecular structure, with the ionic liquid counterions penetrating the ionosilica matrix surrounding the mesopores. The poly(ionic liquid) forms patches decorating the pore walls (see Figure 1), with tunable conformation sensitive to solvent conditions. This behavior is anticipated to be generic in self-assembled ionosilica systems, due to the separation of the ionic liquid from the matrix, while the polymer molecules have affinities for both matrix and ionic liquid.

Keywords: scattering, ionic liquids, template, mesopores, polymer

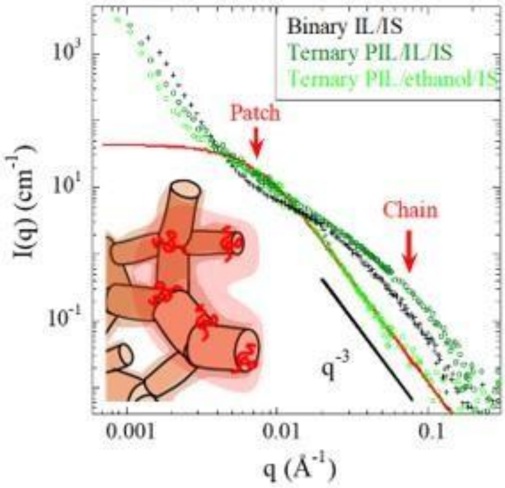

Figure 1. *SANS intensities of binary and ternary (with 2% H/D-PIL) systems, and the same ternary sample after removing IL and impregnation in H/D-ethanol. The red line is a fit using the generalized Debye function, with a high-q exponent of -3 and a Guinier radius of 31 nm...*

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In Situ Monitoring of Soil Removal from Contaminated Model Fabric Films

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The removal of contaminating soils from clothing is an intensive process requiring large quantities of energy and water. Reducing this environmental impact through more effective detergent formulations is a fundamental challenge in the home and personal care industry. This will require a greater understanding of the interactions between soil, fabric, and cleaning formulations. However, in situ monitoring of soil removal during the wash process is extremely challenging. We report a method to study these interactions on model fabric surfaces using FTIR-ATR spectroscopy under flow conditions. By employing derivatives of lipids commonly found on soiled garments specifically labelled with IR-active groups, the removal of individual components from the surface can be monitored, allowing the investigation of stain removal at a chemical level. Our results so far have shown promise, allowing us to establish relative rates of removal of fatty acids and triglycerides. Furthermore, we can rapidly test new washing conditions, for example surfactant composition, or addition of lipases and polymers *in situ*. We anticipate this technique will allow the removal of soil to be probed in detail, enabling the development of more efficient and sustainable detergent formulations.

Keywords: Soil Removal, Surfactant, Lipase, Soil Release Polymer

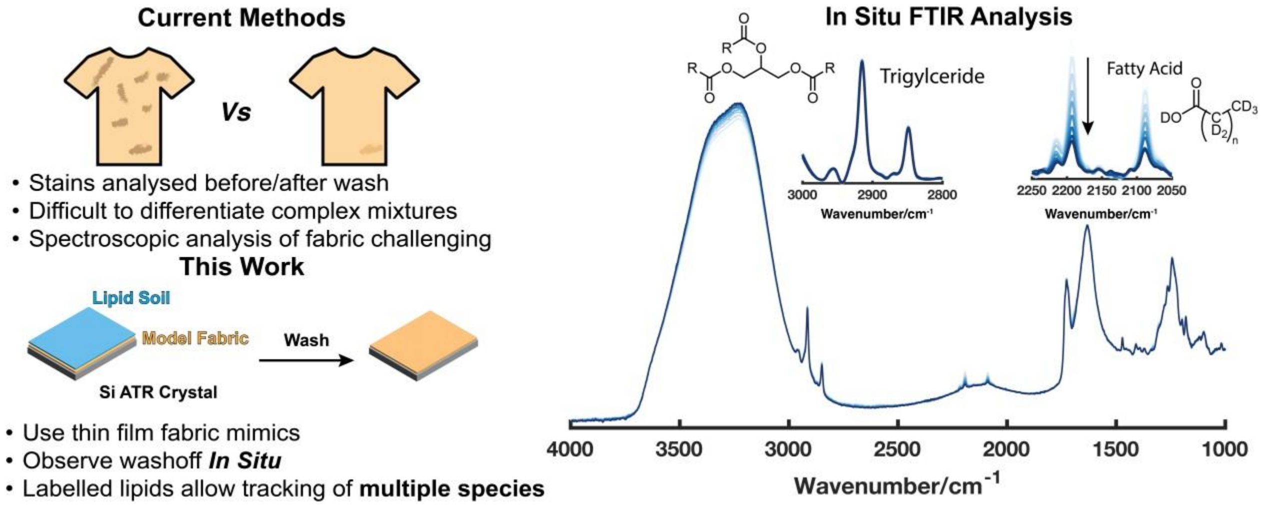

Figure 1. *In Situ FTIR analysis of soil removal from a contaminated model fabric film showing selective wash-off of deuterated fatty acids from a mixture of lipids.*

Controlled Anisotropy in Bicontinuous Emulsions for Passive Cooling

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Temperature rise due to climate change increases the demand for cooling of living spaces. Currently, this cooling demand is primarily met using active cooling, such as air conditioning systems. Passive cooling could meet part of this demand without energy expenditure. Passive radiative cooling can be achieved by tuning the optical properties of a surface in such a manner that it reflects almost all of the incoming solar irradiation[1]. One highly reflective surface found in nature is the shield of the white scarab beetle. The high reflectance of the shield is a result from the anisotropy in its interwoven structure of chitin filaments[2,3].

Bicontinuous interfacially jammed emulsion gels (bijels) consist of a similarly interwoven structure. Bijels self-assemble via interfacial jamming of nanoparticles during spinodal phase separation of two immiscible liquids[4–6]. While the bijel structure is isotropic, recently the typical domain size has been shown to reach down to several hundreds of nanometers, as necessary for interactions with visible light [7,8]. As such, preparing bijels with anisotropic nanostructured domains would be of interest to provide passive cooling.

Here, we present the synthesis of bijels that contain flexible polyacrylamide. By applying a stretching force these bijels are deformed into an anisotropic structure similar to the beetle shield, as shown in Figure 1. We image the structures using confocal laser scanning microscopy and scanning electron microscopy, which allow us to reconstruct a 3d representation of the bijel. We quantify the changes in structure using Minskowski tensors[9], showing that we have control of the anisotropy of bijel structures. In future studies we will use the structural control to experimentally determine the relation between anisotropy and reflectance.

Keywords: Passive cooling, Bicontinuous emulsion gels, Anisotropy

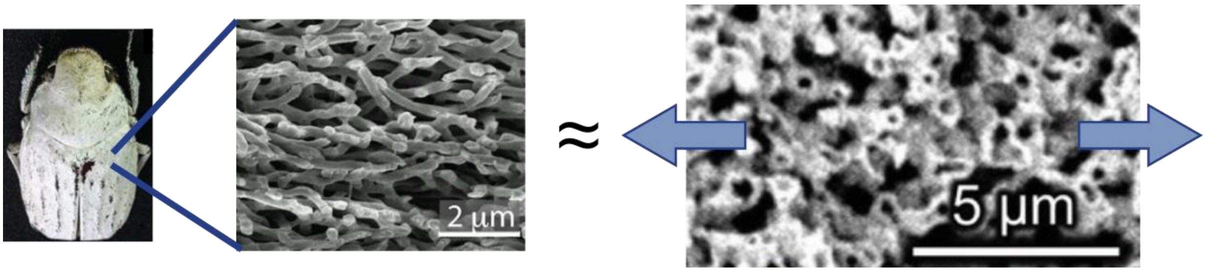

Figure 1. *The structure of the shield of the white scarab beetle (left) can be approximated by stretching a bijel (right). (White scarab beetle and SEM micrograph of shield adapted from [2], bijel SEM micrograph adapted from [7]).*

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Monday 29th September 2025

P. Polymers and Networks

(Room 3)

Using phase separation to fabricate porous hydrogels

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It is surprisingly difficult for water and solutes to move around inside of most hydrogels. For example, dry, cm-thick hydrogel samples can take days to fully swell in water in water, while bulky drug molecules often can't diffuse in or out of many synthetic hydrogels. This is largely due to the small mesh size (typically O(10-100 nm)) of many hydrogels. However, there are many situations where it would be extremely useful to controllably increase the mobility of water or solutes in hydrogels: for example in rapidly-swelling soft actuators or fast-absorbing materials, hydrogels for drug delivery, tissue culture scaffolds, or in selective membranes. To achieve better transport inside hydrogels, a natural solution is introduce additional connected porosity into the hydrogel microstructure.

A powerful technique for introducing porosity in gels is polymerization-induced phase separation (PIPS). This can rapidly produce homogeneous, macroscopic hydrogel samples. However, it is still largely an empirical process that relies on lengthy experimental optimization to create gels with desired properties. Here, we address this by investigating PIPS in a model system consisting of polyethylene glycol diacrylate (PEGDA) and various different solvents. We show that the onset of phase separation is essentially dictated by the overlap concentration of the prepolymer solution. Furthermore, the resulting gel pore structure depends on the physical mechanism that triggers phase separation. The results allow us to quickly identify conditions for creating hydrogels with desired microstructural properties, and we highlight this by producing rapidly-swelling 'super-porous' hydrogels. Our work is not only relevant to PEGDA, but also sheds light onto (often unwanted) phase separation in other, common hydrogels.

Keywords: Hydrogels, phase separation, polymerization, porosity

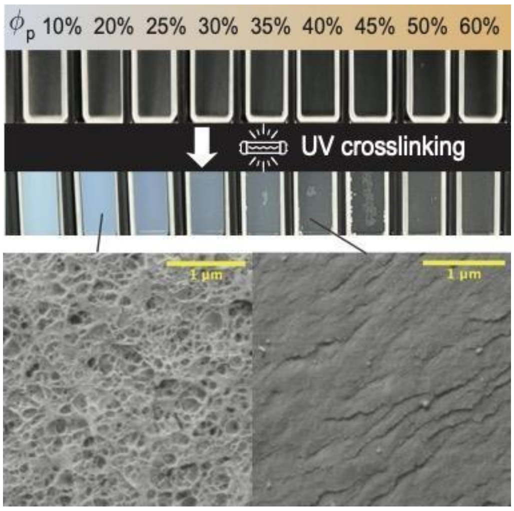

Figure 1. *PEGDA hydrogels created by polymerizing solutions with different polymer contents. Top row: unpolymerized solutions. Bottom row: the resulting polymerized hydrogels. Solutions with lower polymer contents phase separate during polymerization to form porous hydrogels. These porous hydrogels appear cloudy.*

Hydrogels as functional group carriers for selective sensing applications

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Hydrogels – polymer networks that are swollen in an aqueous medium – are extraordinarily useful materials when interaction with an aqueous environment is required. Therefore, hydrogels are popular in diverse and interdisciplinary research activities focused on regenerative medicine, tissue engineering, drug delivery, soft robotics, or sensing, the latter being the focus of the present contribution. The versatility of hydrogels results from the fact that essential properties of hydrogels can be tailored according to the requirements. For adsorption and sensing, especially the relatively easy introduction of functional groups in combination with a typically pronounced mobility of solutes [1], both within the entire hydrogel volume, are crucial. As a result, functional groups for adsorption and concentration enhancement of solutes inside hydrogels are available and accessible. By analysis of a hydrogel property sensitive to the concentration of the solute within the hydrogel, a sensor is obtained.

In this contribution, we highlight the versatility of hydrogels for sensing applications by exploring ways to achieve selective sensing of solutes both by non-specific and specific interactions of hydrogels with the solutes [2, 3]. Especially, we present a novel sensing approach using differently functionalized hydrogels for sensing of multiple solutes simultaneously [4]. We show that our approach enables to selectively and quantitatively measure the concentrations of the drugs diclofenac and metoprolol in aqueous solution based on the hydrogels' conductance, although there are no specific interactions involved. The proposed sensing concept is based solely on the distinct interactions of the functionalized hydrogels with the drugs, depending on the functionalization and the corresponding conductance responses. These interactions are fully described based on physical models, thus introducing a quantitative mathematical framework for the sensing system with the potential to be extended for future use in more complex mixtures.

Keywords: hydrogels, sensors, adsorption, conductance, refractive index

Acknowledgements: Generous funding by the Max Planck Society, the German Research Foundation (grant ID TO 211/4-1), the Carl Zeiss Foundation within the *Projekthaus NanoBioMater*, the University of Stuttgart and the Ministry of Science, Research and Arts of the Federal State of Baden-Württemberg (Germany) within the *Leistungszentrum Mass Personalization* is gratefully acknowledged.

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Associative phase separation in single-step polyelectrolyte complex coatings

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Polyelectrolyte complexes were shown to be promising water-based functional coatings, with, for example, oxygen barrier and flame retardant properties. Usually, they are applied in a multi-step process, where either 1) the substrate is covered alternatingly with positive and negative polyelectrolytes, or 2) the polyelectrolytes are cured in a buffer after application.

In our recent research, we apply polyelectrolyte complexes in a single-step by evaporation of ammonia. Here, evaporation of base from the water-based formulation causes the pH to drop only after application on a substrate. By combining this principle with weak polyelectrolytes, that only get charged after the pH drops, we can selectively but effortlessly "cure" coatings after application.

However, the changing charge density causes both the interaction strength to increase ("curing" the coating), as well as associative phase separation to occur. Understanding and controlling this associative phase separation is crucial to successful application of single-step polyelectrolyte coatings. In this work, we present how we can follow and understand the associative phase separation occurring in the coatings, and show how we can use fluorescence microscopy as an efficient and non-destructive tool for this purpose.

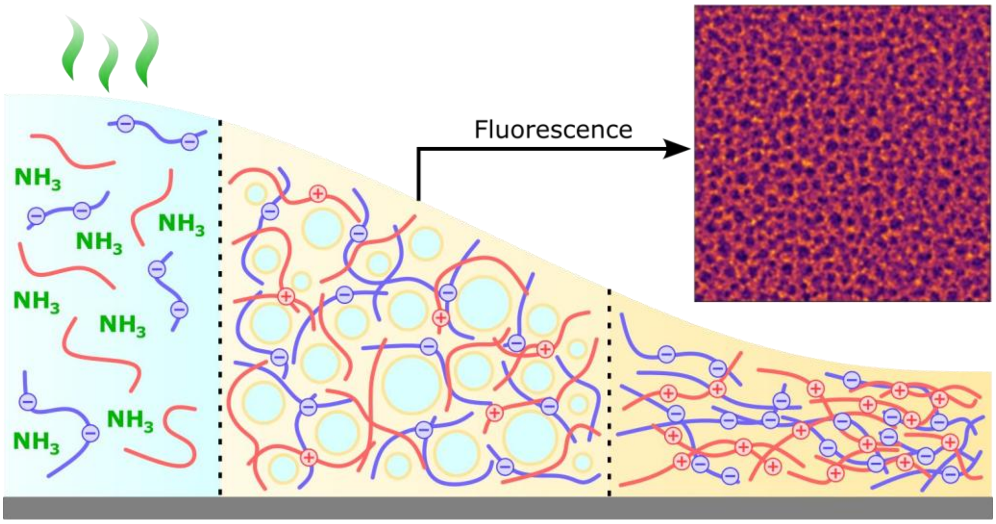

Figure 1: *The formation of a polyelectrolyte complex coating in a single step. By evaporating ammonia from a solution containing weak polyelectrolytes, the polycation gets progressively more charged. This first causes associative phase separation, observable with confocal microscopy, before forming a dense, solid coating.*

Keywords: Polyelectrolytes, phase separation, coatings, microscopy

Acknowledgements: This work is supported by and a part of Advanced Research Center for Chemical Building Blocks, ARC-CBBC, which is co-founded and co-financed by the Dutch Research Council (NWO) and the Netherlands Ministry of Economic Affairs and Climate.

Mechanical assessment of microfluidically-generated poroelastic microgel particles

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Soft microgels have numerous applications across diverse fields, like in tissue engineering as scaffolds, as drug delivery systems, in soft robotics, or for instance as model systems for suspensions or colloids. Among these, photopolymerized hydrogels such as poly(ethylene glycol) diacrylate (PEGDA) have been commonly used due to their highly tunable mechanical properties. However, proper characterisation of these properties is challenging, in part due to their small scale, on the order of tens of microns, and in particular the lack of assessment of their time-dependent properties. Here we provide a comprehensive mechanical characterisation of individual photopolymerised microgels [1,2]. To characterise the mechanical properties we use a combination of approaches: atomic force microscopy (AFM) and nanoindentation for precise local measurements, and a microfluidic technique based on flow-induced deformation for non-contact characterisation.

First, we performed indentation-relaxation tests using AFM and a nanoindenter on PEGDA microdisks immersed in water. By varying indentation depth and probe diameter, we changed the contact area and observed relaxation responses indicative of poroelastic behaviour. In particular, larger contact areas resulted in longer relaxation times. Preliminary results also showed that increasing the amount of solvent increased the relaxation time. Furthermore, while relaxation times were relatively short in water, we anticipate significantly longer relaxation times when these microgels are studied in more viscous environments.

For the second approach, we measure the deformation of a microgel beam fabricated insitu in a microchannel and subjected to a flow [4]. This technique directly provides the Young's modulus of the material and shows potential for further investigation of relaxation behaviours in microgels.

Keywords: poroelasticity, hydrogels, AFM, nanoindenter

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Elastic heterogeneity governs spatial distribution of adsorbed molecules in a soft porous crystal

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Metal–organic frameworks (MOFs), which possess a high degree of crystallinity and a large surface area with tunable inorganic nodes and organic linkers, often exhibit soft mechanics upon molecular adsorption. When guest molecules are adsorbed heterogeneously, heterogeneity in the lattice structure and stiffness of host frameworks—elastic heterogeneity—emerges due to the interaction between guest molecules and host matrices. However, the role of elastic heterogeneity remains elusive.

We show the role of elastic heterogeneity in the adsorption–desorption transition[1]. We construct a minimal model incorporating adsorption-induced lattice expansion/contraction and an increase/decrease in the elastic moduli. In this model, the effective interaction between guest molecules emerges via the host's elasticity. Monte Carlo simulation reveals asymmetric contributions of energy and entropy in the hysteretic nature of adsorption–desorption transition. This is due to the difference in shapes of the adsorbed and desorbed domains (Fig 1), which is understood by Eshelby's inclusion argument. Furthermore, elastic heterogeneity induces spatial patterns, including an adsorption superlattice[2] and surface creasing. Our results provide a theoretical guideline for designing MOFs with tunable adsorption hysteresis and pattern formations of adsorbates using elastic heterogeneity.

Keywords: elastic heterogeneity, soft porous crystals, metal–organic frameworks

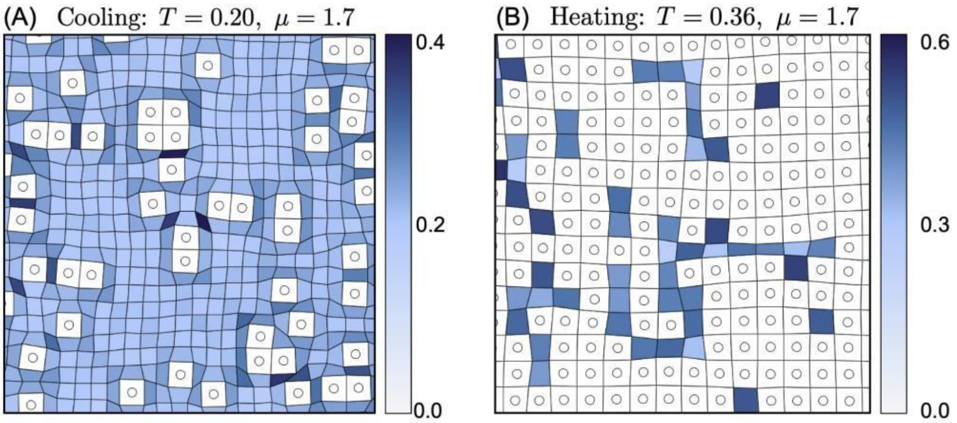

Figure 1. *Heterogeneous distribution of the adsorbates and the elastic energy. (A) Snapshot of a desorbed state slightly above the adsorption transition temperature in the cooling process. (B) An adsorbed state obtained slightly below the desorption transition temperature in the heating process. Circles denote the adsorbed sites. The color in the desorbed sites represents their energy. Reproduced from ref.[1].*

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Harnessing Molecular Architecture for the Design of High-Performance Single-Ion Polymers in Energy Storage

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The development of single-ion solid polymer electrolytes (SI-SPEs) with high ionic conductivity is critical for enabling safe, long-lasting, high-energy-density batteries. However, a key challenge remains: achieving materials that combine a cation transference number near unity with robust mechanical properties—without compromising ionic conductivity. In this work, we present a nanostructured SI-SPE system that addresses this trade-off by incorporating polyanionic nanoparticles into a low-molecular-weight, liquid poly(ethylene oxide) (PEO) matrix. These nanoparticles are composed of poly(styrene-4-sulfonyl(trifluoromethylsulfonyl)imide) lithium (PSTFSILi) arms and ion-conducting PEO arms, forming (PSTFSILi)_n(PEO)_n star-like architectures with $n \approx 22$.This macromolecular design yields well-dispersed particles up to 55 wt%, facilitating the formation of a continuous, nanostructured network of liquid PEO channels that support efficient cation transport. Remarkably, ionic conductivity remains nearly constant—on the order of 10^{-5} S/cm—across the composition range, while the material's shear modulus (G') increases by over five orders of magnitude with increasing nanoparticle content. These results demonstrate a promising strategy for decoupling mechanical strength from ion transport, offering new design principles for SISPEs in next-generation lithium metal batteries.

Keywords: Solid polymer electrolytes, single-ion electrolytes, solid-state batteries

Acknowledgements: Acknowledgements: The research work was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the " RRF: Basic Research Financing (Horizontal support for all Sciences), Sub-action 1. Funding New Researchers –" (Project Number: 15955).

Ελλάδα 2.0 ΕΘΝΙΚΟ ΣΧΕΔΙΟ ΑΝΑΚΑΜΨΗΣ ΚΑΙ ΑΝΘΕΚΤΙΚΟΤΗΤΑΣ
Με τη χρηματοδότηση της Ευρωπαϊκής Ένωσης NextGenerationEU
ΕΛ.Ι.Δ.Ε.Κ. Ελληνικό Ίδρυμα Έρευνας & Καινοτομίας

Molecular Scope: watching macromolecular dynamics at solid-liquid interfaces at the single-chain level

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Molecular-scale interactions between polymers in solution and solid surfaces govern a large number of macroscopic processes in soft matter, from surface functionalization to hydrogel friction. Despite extensive characterization of these processes at the macroscopic level, our molecular understanding of polymer/surface interactions remains scarce, particularly under out-of-equilibrium situations. Here, we couple state-of-the-art single-molecule microscopy techniques with microfluidic transport, to directly track the nanoscale dynamics of single fluorescently tagged PEG macromolecules at solid/liquid interfaces, allowing to probe their subtle couplings with interfacial hydrodynamic flows.

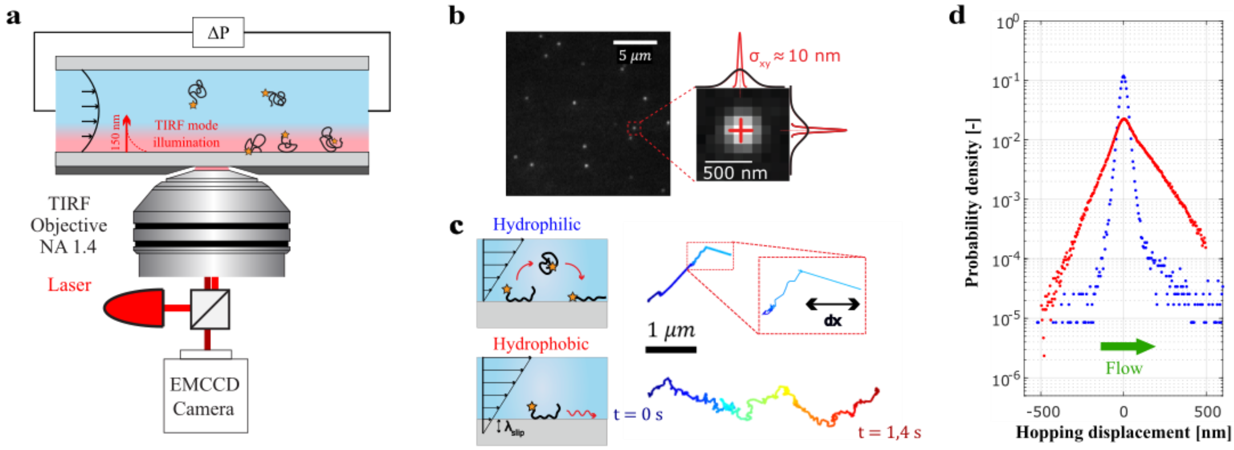

Figure 1: **(a)** Experimental set-up used to probe single-chain dynamics under flow. **(b)** Diffraction-limited spot, allowing for nanometric localization and tracking of the end-grafted fluorophore, i.e., the chain position. **(c)** Representative single-chain trajectories on hydrophobic and hydrophilic surfaces, with the corresponding ensemble single-chain hopping displacements **(d).**

In the absence of hydrodynamic forces, we uncover an heterogeneous and strongly non-Brownian surface diffusion for individual chains, which alternate between a low-mobility adsorbed state and long desorption-mediated jumps through the solvent [1, 2]. The symmetry-breaking effect of the flow leads to a skewed distribution of interfacial displacements, with an unexpected dependence on the nature of the surfaces. On sticky hydrophilic surfaces, the hydrodynamic flow does not affect the chain motion except for an advective effect during solvent-mediated flights. On slippery hydrophobic surfaces, we instead evidence a peculiar regime of mixed macromolecular friction, whereby the adsorbed chain rubs on the solid wall while being continuously dragged by the near-surface hydrodynamic flow, allowing us to finely disentangle chain/wall and chain/solvent frictional molecular interactions. By allowing for direct observations of molecular-scale interfacial dynamics, our approach brings a new molecular vision of macromolecular friction and adsorbate/surface interaction at flowing solid/liquid interfaces.

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Macroscopic membranes of carrageenan and self-assembling peptides

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Three-dimensional (3D) scaffolds for cell culture aim to recreate the extracellular matrix (ECM) of native tissues, yet accurately replicating the complexity and organization of natural tissues remains a significant challenge.[1] Macroscopic membranes formed through the self-assembly of oppositely charged biopolymer and peptide solutions (MMBPs) represent a promising strategy. Initially demonstrated by Stupp *et al.*,[2] MMBPs consisting of peptide-amphiphiles and hyaluronic acid showed hierarchical organization, including a layer of oriented fibers. These membranes can be formed as flat sheets or spherical structures (a.k.a sacs).

Building upon this strategy, our lab previously developed MMBPs from alginate and the βsheet peptide Pro-Lys-(Phe-Lys) 5-Pro (PFK), exhibiting both fully developed hierarchical structures and non-fully developed morphologies lacking perpendicular fibers. However, structural limitations and inadequate mechanical robustness in alginate-based spherical membranes motivated the exploration of alternative polysaccharides.[3]

Carrageenans, naturally derived negatively charged sulfated polysaccharides, have emerged as promising candidates due to their distinct physical and chemical properties compared to alginate.[4] This study introduces a novel approach to fabricating λ- and κ-carrageenan spherical with precisely tunable sizes and mechanical characteristics, utilizing syringe pump-assisted coassembly. Comprehensive physicochemical characterization techniques, including Small-Angle Xray Scattering (SAXS), and microscopy (SEM and confocal microscopy), were employed to understand membrane formation, structure, and stability under various conditions.

This research presents an innovative platform for creating stable and reproducible spherical biomaterials, emphasizing the role of polysaccharide charge density and gelation kinetics in membrane formation. These advancements have significant potential to attract attention in biomaterial research, particularly for applications in tissue engineering and regenerative medicine.

Keywords: self-assembly; Peptide; Carrageenan; SAXS; Hydrogel

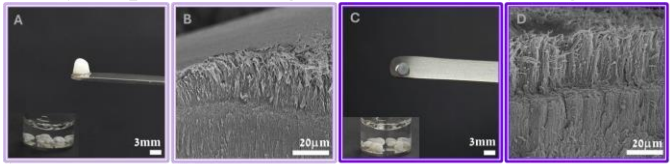

Figure 1. *(A) and (C) show 2 wt% κ-carrageenan/5 wt% PFK micro-sacs at room temperature and 65°C, respectively, while (B) and (D) present their SEM images.*

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Lipase-polymer Conjugates: Synthesis and Catalytic Activity

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The crucial role of enzymes and proteins in key biological processes renders them essential components for the design of advanced hybrid materials engineered to operate under diverse conditions. To address their inherent instability, the synthesis of well-defined enzyme-polymer conjugates has emerged as a promising strategy, particularly for the development of hybrid biomaterials. Recent advances in high-yield techniques, such as oxygen-tolerant controlled radical polymerization and organocatalysis, enable the fabrication of enzyme-polymer conjugates under biologically compatible and mild conditions [1-2]. These hybrid materials, which can be hydrophilic, responsive, or amphiphilic, exhibit unique assembly behaviors with extensive potential applications.

The synthesis of novel pH- and temperature-responsive lipase-polymer conjugates and their catalytic profiles at both the supramolecular and single-nanoparticle level will be presented [2-3]. In contrast to ensemble measurements, single nanoparticle analysis revealed enhanced enzymatic activity of the biohybrids and a well-controlled temperature- or pH-responsive regulation of activity. For the first time, a relationship between nanoparticle size and catalytic performance was observed, with smaller nanoparticles displaying higher catalytic activity and remarkable long-term stability, highlighting their potential in biocatalysis and sustainable industrial applications.

Keywords: protein-polymer conjugates, assembly, catalysis

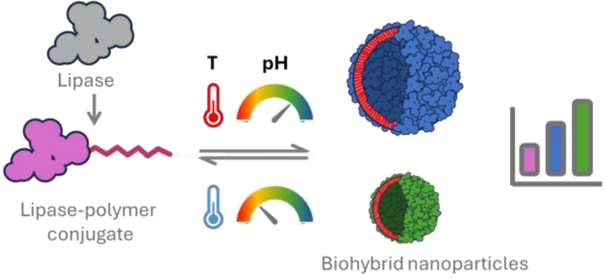

Figure 1. *Assembly dependent enzymatic activity of lipase-polymer conjugates.*

Acknowledgements: The authors acknowledge the Hellenic Foundation for Research and Innovation (HFRI) ΕΛΙΔΕΚ program for funding under the 4th Call for HFRI PhD Fellowships (Fellowship Number: 11118).

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Understanding Poly(acrylic acid)-Lysozyme Association via Molecular Simulations across Different Conditions

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Studying protein-polymer complexes at the molecular level is crucial for understanding how polymers interact with proteins, affecting their stability and function. The complexation process of Lysozyme (LYZ) and poly(acrylic acid) (PAA) is highly dependent on pH and temperature, affecting both the stability and binding dynamics of the interaction network. Using atomistic molecular dynamics simulations, we explored how these environmental factors shape the binding strength, molecular rearrangements, and conformational adaptability of the [LYZ-PAA] complexes. The energetic results reveal that pH has a pronounced effect on the resulting complexes, where higher pH disrupts protein-polymer interactions due to increased electrostatic repulsion, weakening complex formation. At the same time, increase in temperature and thus in molecular mobility, lead to more transient and fluctuating interactions while maintaining overall binding stability. Structural analysis further supports these trends, showing that higher temperatures promote flexibility, while higher pH leads to greater conformational expansion and reduced stability. Through association rate calculations and hydrogen bonding analysis, we identified key residues, such as arginine and lysine, which dominate in the LYZ/PAA interaction at lower pH levels, while higher pH values promote a shift toward hydrophobic interactions. Our findings provide the pH and temperature's crucial role in protein-polymer complexation, offering valuable insights in biomaterials design.

Keywords: Lysozyme, Poly(acrylicacid), Molecular Dynamics, Complexation, Temperature, pH

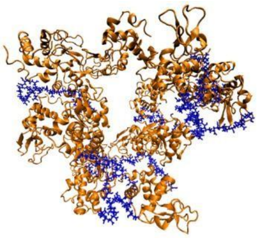

Figure 1. *Representative snapshot of protein-polymer bridges in [LYZ-PAA] complexes.*

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Hyper-Auxeticity and the Volume Phase Transition of Polymer Gels

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Thermoresponsive hydrogels, such as poly(N-isopropylacrylamide) (pNIPAM) networks, exhibit a Volume Phase Transition (VPT) marked by abrupt deswelling and frequently overlooked anomalous auxetic responses (negative Poisson's ratio, ν). While experiments associate VPT with ν minima [1], classical Flory-Huggins theory predicts positive ν [2], creating a critical unresolved discrepancy.

Through advanced numerical simulations of equilibrium and deformed polymer networks, we uncover a Hyper-Auxetic Transition (HAT) at $\nu = -1$, occurring under low crosslinker concentrations (c) and variable temperatures (T) and corresponding to the limit for the mechanical stability of a solid [3]. This exotic mechanical response coincides with a thermodynamic criticality, distinct from the solvent-driven VPT. Crucially, HAT is confined to $c \leq 3\%$, while VPT persists across all c at fixed T, resolving their conflation in prior studies. Phase diagram analyses elucidate the distinct origins of the VPT and HAT: while the VPT is driven by temperature-induced phase separation of polymer chains, the HAT emerges from mechanical instabilities caused by attraction-mediated network buckling under tension. Simulations of low-crosslinked hydrogels (e.g., $c = 1\%$) reveal a striking spatial decoupling between these transitions, with the HAT localized to critical tension regimes and the VPT occurring independently under thermal collapse.

These findings disentangle the interplay between thermal collapse and hyper-auxeticity, offering mechanical insights into the thermo-mechanical duality of hydrogels. By establishing HAT as a distinct critical phenomenon, this work challenges existing paradigms and guides the design of hydrogels with tailored auxetic functionalities for soft robotics, biomedicine, and smart materials.

Keywords: Hydrogels, Auxetic material, Volume Phase Transition

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Exploring the static and dynamical properties of ultra-polydisperse linear polymer solutions

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Polymers used in daily life have intrinsic polydispersity in the molecular weight (MW) that determine the rheology of polymer solutions. The MW polydispersity, often quantified using polydispersity index (PDI = M_w/M_n), is known to impact the rheological behavior [1]. However, PDI is insufficient for fully describing the diverse polydisperse systems and in fact we cannot predict and regulate the solution rheology by changing the molecular weight dispersity.

In this study, we used a polydisperse polymer solution where the polymer's MW obeys a power low with an exponent, *a*. Unlike the PDI, we can express the super polydisperse systems with various "*a*" value. By using a linear polyethylene glycol (PEG), we prepared PEG solutions with *MW* follows a power-law (M^{-a}) (Fig. 1a). By systematically varying the *a* and the maximum $M_{\max}$, we explored their rheological properties under shear flow. Notably, we observed that the overlap concentration $c^{\dagger}$ does not depend on the polydispersity, but the critical (zero-shear viscosity crossover) concentration c^{*} increases in $1 < a < 2$ (Fig. 1b), consistent with trends observed in polydisperse circular particle systems [2]. By using this system, we successfully constructed a phase diagram illustrating the shear-thinning condition (Fig.1c). This diagram shows that the higher polydisperse system has a weaker molecular entanglements, and the lower structural relaxation time. This suggests that polydisperse linear polymers are stretched more under shear than monodisperse ones. This prediction is also confirmed by the coarse-grained MD simulations of polydisperse linear polymer solutions under steady shear conditions. In summary, we quantitatively clarified the effect of molecular weight polydispersity on the rheological properties of polymer solutions whose molecular weights follow a power-law distribution. The zero-shear viscosity can be described by an equation that considers the power-law exponent *a*. In addition, the shear thinning under shear can be described by the power-law exponent *a* and $M_{\max}$.

Keywords: Polymer, Polydispersity, Rheology, Shear thinning

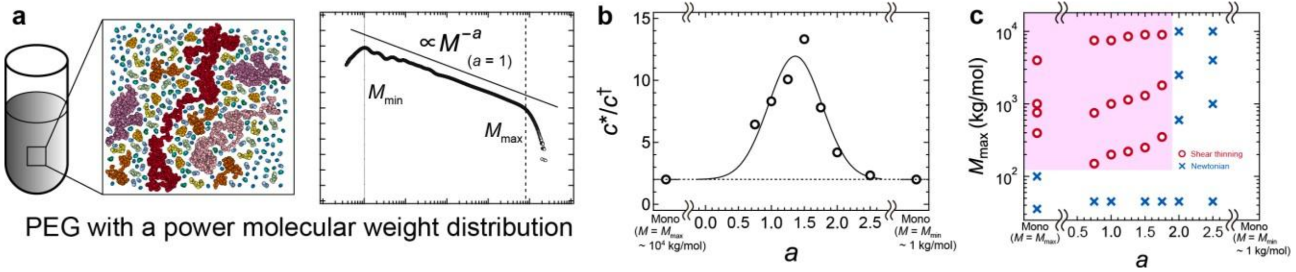

Figure 1. *(a) Schematic of PEG with power-law MWD (left), and the MWD actually produced in our experiments (right). (b) Critical (zero-shear viscosity crossover) conc. c^* normalized by overlap conc. $c^\dagger$ as a function of the powerlaw exponent a. (c) Phase diagram illustrating the shear-thinning behavior ($a < 2$ and $M_{\max} > 10^2$ kg/mol).*

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Homogeneous and Heterogeneous Cluster Formation in Mixtures of Ester and Hydroxy-Terminated cis-1,4-Polyisoprene Chains in Natural Rubber

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The terminal structures of cis-1,4-polyisoprene (PI) chains significantly influence the exceptional mechanical properties of Hevea natural rubber (NR), including high toughness, wet skid resistance, and strain-induced crystallization. We conducted all-atom molecular dynamics simulations to investigate the structural and dynamic properties of PI melt systems with various terminal group combinations. These included single-component melts and binary mixtures of chains with ester- and hydroxy terminated α-terminal groups. The study revealed that hydrogen bonding between αterminal groups drive the formation of stable homogeneous and heterogeneous clusters. In singlecomponent systems, hydroxy-terminal groups promoted homogeneous clusters, while in binary mixtures, heterogeneous clusters formed between ester and hydroxy terminals. These clusters, ranging in size from 2 to 5 chains, serve as physical junction points, slowing chain dynamics and enhancing network stability. Dynamic properties, such as rotational relaxation, Rouse mode times, and stress–stress autocorrelation, were significantly influenced by cluster formation, particularly in mixed systems. The stress–stress autocorrelation function, $G(t)$, exhibits a Rouse-type relaxation behavior ($G(t) \sim t^{-1/2}$) in the intermediate time range for PI0. In contrast, the mixed melt systems PI0 show a slower relaxation compared to the pure components. This slower relaxation is attributed to the formation of stable, well-ordered heterogeneous clusters, driven by hydrogen bonding between ester and hydroxy-terminal groups. These findings provide evidence for the formation of physical junction points between hydroxy- and ester-terminated polyisoprene chains through their respective α1, α2, α3, α4, α5, and α6 terminals. These physical junction points might be crucial for superior properties of NR such as high toughness, crack growth resistance, and strain induced crystallization.

Keywords: Natural Rubber, All Atom Molecular Dynamics, cis-1,4-polyisoprene, terminal ends

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Neutron Investigations on the Structure and dynamics of ringlinear polymer blends

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Blends of ring and linear polymers pose fascinating challenges. While in such blends the dynamics of linear chains is hardly affected, already minute concentrations of linear chains have a large effect on ring rheology /1/. Blends of rings with linear chains are characterized by strong interpenetration of the rings by the linear chains. These threadings swell the ring conformation significantly and alter the ring dynamics very strongly, as large scale ring motions are only possible by constraint release of the linear component /2/. We have performed systematic Small Angle Neutron Scattering (SANS) investigation of such blends, where we have varied the ring volume fraction ϕ_R for a ring 40 kg/mol polyethylene-oxide (PEO) in a linear matrix of 100 kg/mol. We found that with increasing ring fraction the ring radius of gyration (R_g) swells by more than 20% . At the same time the fractal dimension, which is close to a Gaussian conformation at low ϕ_R, decreases to the value of the ring melt. Following a random phase approximation (RPA) treatment, the Flory-Huggins parameter (χ_F) is large, negative and independent of ϕ_R, signifying ring-linear attraction leading to ringring repulsion /3/. Concerning the ring dynamics in symmetric ring/linear blends of 40kg/mol PEO as a function of ϕ_R we observed a transformation of typical self-similar ring relaxation to local reptation type dynamics at higher linear fraction, where the motion of the ring is slaved by the linear host. The cross-over between the two types of motions takes place for 0.25 <ϕ_R<0.5. Even though at ϕ_R=0.5 the characteristic spectral shape assumes the local reptation scheme, the actual constraints expressed by the apparent entanglement length Ne are less than those at higher linear volume fraction (N_e≅100 compared to N_e≅70 for ϕ_R≤0.35. In addition ring mode suppression is observed: A detailed mode analysis of the neat ring melt as well as the ϕ_(R)=0.95 blend revealed a suppression of the first ring p = 2 mode. For ϕ_(R)=0.75 also the second ring mode p = 4 is suppressed. The p = 2 mode length scale comprises the full ring size; it suppression already in the neat melt indicates significant constraints on the ring motion beyond the self-similar mode structure. This observation correlates with the non- exponential decal of dynamic shear modulus at long times, which is attributed to ring-ring threading.

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Vitrimer-like Behavior in Main-Chain Poly(ionic liquid) Elastomers via Anion-Tuned Crosslinking

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Thermosetting resins are known for their excellent heat and creep resistance, outperforming thermoplastic resins in these aspects. Nevertheless, their irreversibly crosslinked network structure poses a major challenge for recycling and reshaping. With increasing interest in environmental sustainability, there is a growing demand for crosslinked polymer materials that can be reprocessed. In this context, vitrimer-type elastomers—capable of dynamic bond exchange without altering the overall crosslink density—have attracted significant attention. Despite growing interest, the development of ion-conductive vitrimers still remains limited.

In this study, we report the preparation and characterization of ion conductive vitrimer-like main-chain poly(ionic liquid) (TPIL) elastomers featuring dynamic behavior through anion-tuned crosslinking. The TPILs were prepared by thermal click polymerization of clickable imidazoliumbased ionic liquid monomers[1], followed by crosslinking via *N*-alkylation with dihalogenated crosslinkers. Two types of anions—iodide (I^-) and bis(trifluoromethanesulfonyl)imide ($TFSI^-$)— were incorporated into the crosslinking units to evaluate their influence on material properties. Rheological analyses revealed that TPIL elastomers with I^- crosslinkers exhibited rapid stress relaxation, which fitted well with the Kohlrausch-Williams-Watts model[2], indicating vitrimer-like dynamic behavior. In contrast, their $TFSI^-$-based counterparts showed negligible relaxation. Furthermore, thermal reshaping was only achievable for elastomers containing I^-, further confirming the presence of vitrimeric characteristics induced by this specific anion. These findings demonstrate that the vitrimeric nature of TPIL elastomers can be effectively tuned through anion selection in the crosslinker, offering a new design strategy for ion-conductive and reprocessable polymer networks.

Keywords: Poly(ionic liquid), Vitrimer, Dynamic covalent networks, Stress relaxation, Anion

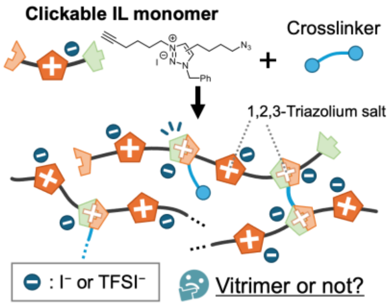

Figure 1. *Schematic image of TPIL elastomers with different crosslinkers.*

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The Phase Stability of Interpenetrated Dual Polymer Networks with Orthogonal Reversible Bonds

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We explore the phase behaviour of binary mixtures of associative polymer chains with two orthogonal reversible bonding mechanisms which connect to a system-spanning cluster upon reaching a certain concentration. For this purpose, we perform molecular dynamics simulations using both a full-monomeric model (AM) that takes account of monomer-resolved interactions, and the effective fluid model (EFL) which is a coarse-grained approach based on the potential of mean force (PMF). It has been shown [1] that a binary mixture of polymers with two orthogonal reversible bonding mechanisms and only one type of reactive site per chain is not stable at concentrations higher than the overlap and undergoes phase separation. We probe the possibility of exchanging a small fraction of reactive sites with their orthogonal equivalent and investigate which impact their position within the linear polymer has on the PMF and their phase stability. We combine the simulations of the AM and EFL models together with theoretical phase diagrams to conclude that the two components of polymers form mixed dual networks which are resistant to phase separation even at high concentrations (Fig. 1), provided that the minority sites are not placed into close vicinity to each other to avoid the formation of intramolecular loops but rather facilitate intermolecular bonds between the components. We are further investigating the behaviour of the dual polymer networks under shear flow and the influence of the reversible bond strength.

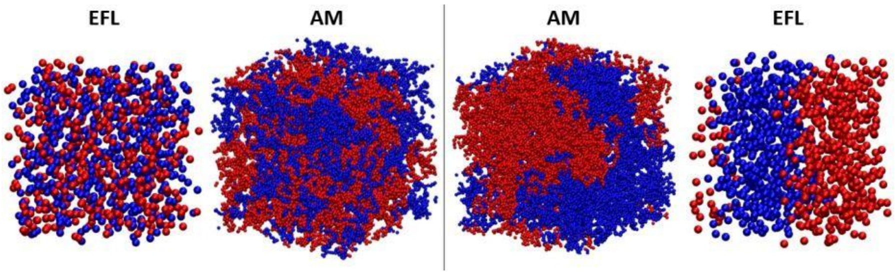

Figure 1. *Snapshots of 50/50 mixtures of polymer chains with reversible bonds as explained in the text and coloured in two different colours. Full monomer (AM) model in center, effective fluid model (EFL) in the corners. Left: Placing the minority reactive sites on the chain ends stabilizes the two mixed dual networks even at concentrations far over the overlap.*
Right: In contrast, placing them in the chain centers close to each other results in phase separation at high concentrations.

Keywords: Molecular dynamics simulations, associative polymers, dual polymer networks, phase separation, shear flow

Acknowledgements: We acknowledge the projects QLUSTER (EU, HORIZON-MSCA-2021-DN01-GA101072964), PID2021-123438NB-I00 (MCIN/AEI/10.13039/501100011033, ERDF A way of making Europe) and IT1566-22 (Basque Government).

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Mechanochemical Molecules to Understand Crack Initiation in Soft Polymer Networks

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Tough soft materials such as multiple network elastomers (MNE)[1] or filled elastomers are typically stretchable and include significant energy dissipation mechanisms that prevent or delay crack growth. Yet most studies and fracture models focus on steady-state propagation. We report an in situ spatial- temporally resolved 3D measurement of molecular damage in mechanophore-labeled MNE just before a crack propagates. This technique, complemented by digital image correlation, allows us to compare the spatial distribution of both damage and deformation in single network (SN) elastomers and in MNE[2]. Compared to SN, MNE have a widespread damage in front of the crack and, surprisingly, delocalize strain concentration. Additional measurements of time dependent molecular damage during fixed grips relaxation in the presence of a crack reveal that the less localized damage distribution delays fracture initiation. While SN follow well the picture of Lake and Thomas with a localized damage at the crack tip systematically leading to crack advance, the MNE, representative of tough elastomers, do not. We clearly observe that TN elastomers form a large molecular damage zone (see Figure 1) that is much more diffuse around the crack tip. As the load is increased or maintained constant, the molecular damage increases but the stress and strain fields become less singular and do not necessarily lead to crack propagation but to a blunting of the crack. At very high applied stress when the damage is extensive, a fast propagation occurs in a highly damaged zone.

Keywords: elastomer, network, fracture, mechanochemistry

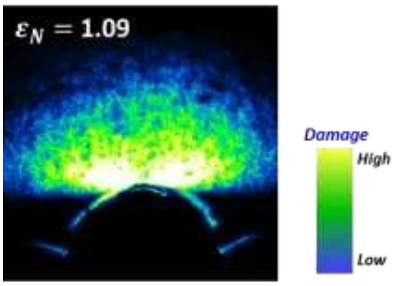

Figure 1. *3D damage map of fluorescence intensity by confocal microscopy, in a triple network at a strain of 109%.*

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Effects of elasticity on phase separation in polymer networks

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Phase separation in gels has been studied for decades, but has received renewed importance in recent years because of its potential role in controlling biomolecular liquid condensates that form in elastic media such as the chromatic matrix of eukaryotic cell nuclei. We study the effects of polymer elasticity on phase separation in gels and identify several features that have not been addressed concretely, despite the decades of research: (1) The long range nature of elastic interactions implies that, in many cases, the energy function of a deformed medium is non-extensive, which in turn implies that the usual common tangent construction cannot be used to calculate phase equilibria; (2) In constricted geometries one can use the constriction length (the thickness of a plate or the diameter of a rod) to avoid the complications of (non-local) elasticity; (3) Even if one ignores the long-range nature of elasticity, the usual neo-Hookean model of crosslinked polymer networks cannot give rise to phase equilibria in many, if not most, cases, and one must use more realistic strain-stiffening models. We will relate these points to recent experiments on phase separation in swollen polymer networks.

Keywords: Non-extensive thermodynamics, polymer gels, phase separation, rubber elasticity, gel swelling

Monday 29th September 2025

F. Fluid Dynamics and Rheology

(Room 4)

Transition to turbulence in conduits with compliant walls

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Experiments on the flow through conduits (channels and tubes) with compliant walls have been carried out in micro-channels of height (minimum dimension) in the range 1.5 mm to 100 microns with compliant walls as shown in figure 1 (left). These are prepared as cylindrical or rectangular bores in blocks of polydimethylsiloxane (PDMS) or polyacrylamide gels using template assisted soft lithography.

The elasticity modulus of the gel walls is in the range of 17-500 kPa for PDMS, and as low as 1 kPa for polyacrylamide gels. These measurements show that there is an instability of the laminar flow and a transition to a flow with intense cross-stream mixing when the Reynolds number exceeds a critical value that depends on the elasticity of the wall material. The Reynolds number is as low as 500 for a pipe of diameter 1 mm, and as low as 100 for a channel of height 100 μm[1]. Large fluctuations are observed in the cross-stream velocity in the dye-stream experiments, and the time for complete cross-stream mixing smaller, by a factor of 10^5, in comparison to diffusion in a laminar flow[2].

At a Reynolds number in the range 200-400 in a channel of height 100μm, the root mean square of the velocity, when scaled by the average flow velocity, is comparable to that in a rigid channel at a much higher Reynolds number of 10,000. The characteristics of the velocity fluctuations are different from those in a rigid channel, because of the possibility of wall motion in a compliant surface. The stream-wise velocity fluctuation has a maximum at the wall, in contrast to the near-wall maximum in a rigid channel. There is a significant non-zero Reynolds stress at the wall. The energy production rate has a maximum at the wall, in contrast to the near-wall maximum for a rigid surface.

Keywords: Instability, transition, compliant wall.

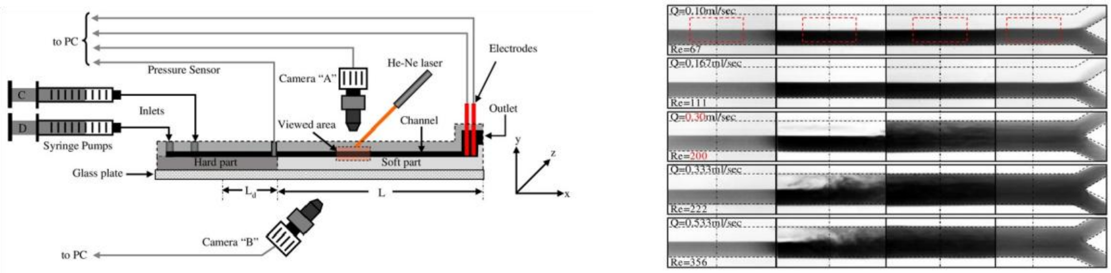

Figure 1. *Experimental apparatus for transition and turbulence in a channel with compliant walls (left), and transition in a microchannel of height 100 μm at Reynolds number 200.*

Acknowledgements: The author thanks the Department of Science and Technology, Government of India for financial support.

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Flow of non-Brownian suspensions under power ultrasound

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The flow behavior of non-Brownian suspensions is governed by the interactions between suspended particles. Unlike Brownian suspensions, where thermal fluctuations play a dominant role, non-Brownian suspensions are characterized by the predominance of hydrodynamic and contact forces. At high volume fractions, particle contacts become the primary factor controlling the suspension's viscosity. Frictional contacts, in particular, can lead to dramatic increases in viscosity, sometimes resulting in discontinuous shear thickening. To control or modify these contact interactions, some researchers propose the use of mechanical vibrations or ultrasound.

In this study, we revisit this question in slightly shear-thinning suspensions of polystyrene beads in silicone oil. Using microfluidic devices, we simultaneously probe particle concentration and rheological properties. Our results reveal a viscosity decrease when ultrasound is applied. Surprisingly, this reduction is linked to particle aggregation under ultrasound, forming alternating regions of higher and lower particle volume fractions. These regions arise as particles migrate toward low-pressure zones (antinodes) due to acoustic radiation forces, which result from differences in acoustic impedance between the particles and the surrounding fluid. Consequently, the flow becomes more heterogeneous and fluid due to the presence of these diluted zones.

Interestingly, in our study, the viscosity reduction is not due to the disappearance of particle contacts but rather to the formation of highly concentrated zones with numerous contacts and solid-like regions, coexisting with highly fluid zones.

Keywords: Ultrasound, Particles, Contact

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Inverse Leidenfrost impacting viscoplastic drop

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We study the spreading of ambient-temperature millimetric/centimetric viscoplastic drops after impacting a quartz plate covered with liquid nitrogen. As the drop expands, nitrogen evaporates, creating a vapor film that levitates the drop, leading to inverse Leidenfrost conditions. The drops are modeled as Herschel-Bulkely fluids. Three spreading regimes are observed, under negligible capillary effects: (I) inertio-plastic, (II) inertio-viscous, and (III) inertio-visco-plastic. In all spreading regimes observed, the vapor film has marginal effect, with the dissipation dominated by bi-axial extensional deformations. However, these regimes are strongly influenced by the initial aspect ratio of the drops, indicating that drop shape can be used to control spreading behavior. The study combines experiments and three-dimensional numerical simulations, analyzing spreading dynamics through scaling laws and a dimensionless parameter linking maximum spreading to the observed regimes.

Keywords: drops; impact; inverse Leidenfrost; experiments: numerical simulations

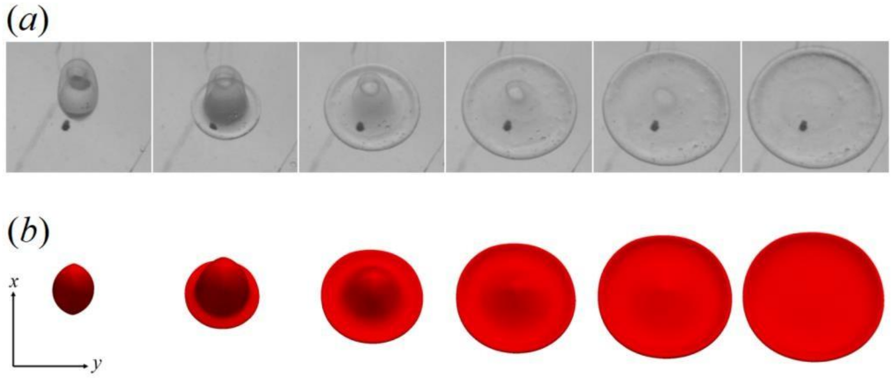

Figure 1. *Snapshots: a viscoplastic Carbopol drop spreading under inverse Leidenfrost conditions. (a) Experiments. (b) 3D numerical simulations.*

Acknowledgements: The authors would like to acknowledge the support from the UCA$^{\text{JEDI}}$ program (IDEX of Université Côte d'Azur), the PSL Research University under the program `Investisse- ments d'Avenir' launched by the French Government and implemented by the French National Research Agency (ANR) with the reference ANR-10-IDEX-0001-02 PSL. Financial support for this work from the French National Research Agency (ANR) un- der the `Investissements d'Avenir' program (INNpact project, no. ANR-21-CE06-0036) and the H2020 Program (Marie Curie Actions) of the European Innovative Training Net- works (H2020-MSCA-ITN-2017) under DoDyNet REA Grant Agreement (GA) number 765811 is gratefully acknowledged.

Complex Morphology on the Underside of a Leidenfrost- levitated Hydrogel Sphere

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When a liquid droplet approaches a hot surface, vaporization can become sufficient to cause the drop to levitate—this is the Leidenfrost effect [1]. Vaporizable soft solids, e.g., hydrogels, can also exhibit levitation [2] or, in addition, a sustained bouncing effect [3]. In the case of floating liquids, the balance of vapor pressure and surface tension creates an inversion of the curvature on the droplet underbelly. Naively, one might expect that with a levitating soft solid, vapor pressure and elasticity should create a similar equilibrium with a similar curvature inversion. We employ high- speed interferometric imaging [4] to uncover the evolution of a floating hydrogel sphere in contact with a vapor layer. During the transition to the floating state, the hydrogel undergoes three distinct stages. Initially, there is a brief inversion of curvature, highlighting the interplay between elasticity and vapor pressure. Subsequently, the bubble beneath the hydrogel is unable to remain trapped due to mass loss during vaporization, leading to oscillations on the hydrogel's underside. Finally, and contrary to intuition, the contact area stabilizes without any further curvature inversion Fig.1.

Keywords: Leidenfrost effect, hydrogels, lubrication theory.

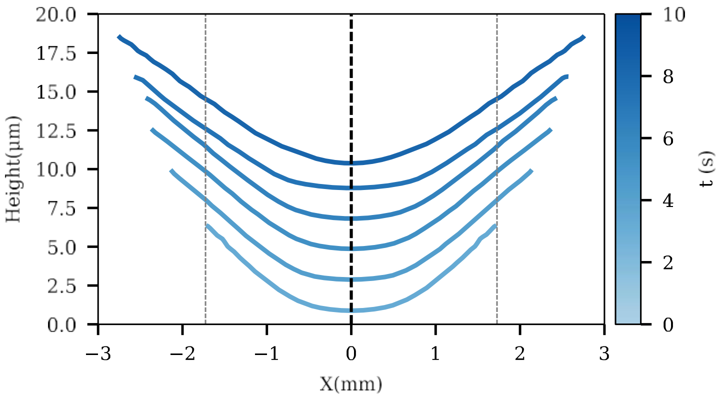

Figure 1. *Reconstructed height profile of the hydrogel underside as indicated for different times*

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Preventing the sinking of a disk by leveraging the boundary jump phenomenon

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Although it is commonly expected that a metal disk placed on the surface of water will sink, our investigation has revealed a surprising phenomenon: a vertical jet directed onto the disk from above can allow it to remain afloat, as shown in **Figure 1**. This counterintuitive result challenges the assumption that the jet's impact would force the disk downward.

We found that this flotation occurs due to water being displaced from the top of the disk by the incoming jet, through a mechanism analogous to the hydraulic jump. This displacement generates a hydrostatic pressure difference, producing an upward buoyancy force that can counteract gravity. Unlike the classical case, the jump radius here is fixed by the disk's geometric parameters—a phenomenon we refer to as a *boundary jump*.

Experimental observations showed that as the disk's submersion depth increases, a transition occurs between two distinct flow regimes (see https://youtu.be/as0wRQj1Zws), reminiscent of those reported by Bush et al. [1]. To analyze this behavior, we developed a theoretical model based on scaling laws, which predicts the submersion depth at which the flow transition occurs. The dimensionless scaling constant was determined through an independent experiment.

As a final step, we performed flotation and sinking experiments, which demonstrated good agreement with the proposed flotation theory [2].

Keywords: Hydraulic Jump, Jets, Thin films, Wakes

Figure 1. *Photograph of a disk floating on the water surface with a vertical jet directed onto it. The disk remains stably afloat over an extended period of time.*

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Importance of dissolved gas transfers around antibubbles

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An antibubble is spherical thin film of gas, surrounded by a liquid, that encapsulates a liquid droplet. Since the hydrostatic pressure is higher at the bottom of the film than at the top, a gravitational gas flow occurs from bottom to top. This process leads to the appearance of thinner, more fragile, film portions and eventually to the nucleation of a hole and subsequent collapse of the antibubble. The thinning dynamics therefore determine the stability of antibubbles. These dynamics were shown to depend both on interfacial rheological properties and dissolved gas transfers between the gas film and surrounding liquid [1].

We present an original method to measure the absolute thickness profile of the antibubble from transmitted monochromatic light, without the need for a reference for the interference order [2]. We use this method to show that antibubbles' thinning dynamics are primarily determined by gas transfers and not by the rheological properties of their interfaces. To better quantify this process, we design the antibubble column, an instrument that allows measuring the dissolved gas mass transfer coefficient, based on the acceleration of antibubbles as they ascend in a liquid. The mass transfer coefficient is shown to depend significantly on the type and concentration of surfactants used to generate the antibubbles.

This measurement is possible because antibubbles are gas-carrying, yet essentially incompressible objects, with a very high surface over gas volume ratio and low-density contrast with the surrounding liquid as compared to bubbles. All these properties are then used to show that antibubbles transfer at least 10 times more gas with the surrounding liquid than a bubble that would carry the same initial amount of gas. Overall, these results show that antibubbles could be advantageously used in liquid/gas reactors [3].

Keywords: antibubbles, interferometry, thin film, drainage, mass transfer, surfactants

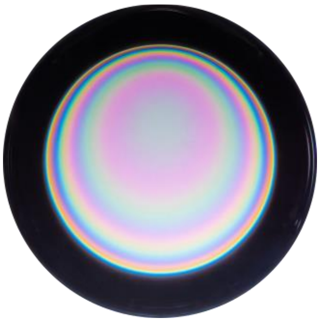

Figure 1. *An antibubble observed in transmitted white light with an RGB photo camera. The diameter of the object is approximately one centimeter.*

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Stokesian Processes: A Physics-Informed Probabilistic Machine Learning Framework for Stokes Flows

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Stokes or low-Reynolds number flows are characteristic of flows at small scales (e.g., biological flows) and/or of high-viscosity fluids (e.g., high-molecular weight polymer melts), making them fundamental to understand a wide variety of physical and biological processes. Unfortunately, standard numerical methods are ill-suited to analyze experimental systems, which are typically characterized by noisy/sparse data, unknown boundary conditions, complex host fluids, etc. In this context, Machine-Learning methods offer a promising alternative, however, most work has focused on high-Reynolds number (turbulent) flows [1].

Recently, we have developed a physics-informed (Bayesian) probabilistic machine-learning framework for solving arbitrary Stokes flow problems, referred to as *Stokesian Processes* (SP) [2]. SP are a form of physics-informed Gaussian Processes (GP) [3], which provide a probability distribution over functions, and which exactly encode the relevant physical laws (i.e., Stokes and continuity equations) into the GP kernels. The SP solution to a generic Stokes flow problem is then obtained as a conditional probability distribution (conditioned on the prior information and all known data), which can be computed exactly. Thus, our SP method outperforms standard deeplearning approaches, e.g., physics-informed neural networks or neural-operators, as it exactly encodes the physics, providing more robust predictions (together with uncertainty estimates), and is less expensive to train.

The original SP method was formulated for simple 2D flows [2]. In this work, we consider extensions to 3D flows and complex (moving) boundaries, as well as experimental applications, e.g., analyzing Particle-Image Velocimetry (PIV) measurements to reconstruct 3D flows/boundary conditions from partial and noisy data.

Keywords: Physics-Informed Machine Learning, Gaussian Processes, Stokes Flow

Acknowledgements: This work was supported by the Grants-in-Aid for Scientific Research (JSPS Kakenhi) under Grant No. 23H04508. We acknowledge the 'Joint Usage/Research Center for Interdisciplinary Large-scale Information Infrastructures' and 'High Performance Computing Infrastructure' in Japan (ProjectIDs: jh230061 and jh240063) for providing the computational resources Wisteria/BDEC-01 at the Information Technology Center, University of Tokyo.

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Jets and waves in gelatin from a cavitation bubble

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The cavitation bubble collapses near a free surface by jetting away from it. Within a certain range of stand-off distances from the free boundary, a "Bullet-jet" is created [1]. This jet reaches a velocity of 40 m/s and travels distances of more than 15 times the maximum radius of the laser-induced cavity before losing momentum. This study reports the experimental observation of how this jet penetrates a block of gelatin (Fig. 1(a)). A theoretical model is constructed by equating the jet's kinetic energy to the gel's elastic energy, expressing the penetration depth in terms of jet velocity, jet diameter, and gel elastic modulus. The calculated prediction matches the experimental results very well (Fig. 1(b)).

It is known that the non-symmetrical collapse of a cavitation bubble creates shear waves in the elastic medium [2]. We use a high-speed polarization camera (CRYSTA PI-5WP, Photron Inc) to visualize the stress field generated in the gelatin as the "Bullet-jet" penetrates the gel. We also vary the bubble stand-off distances and the water height above the gelatin to study how these parameters affect the generation, development, and propagation of shear waves.

In conclusion, this study may be useful for understanding bubble-generated jets for applications such as needle-free injection and flow in viscoelastic media.

Keywords: cavitation bubble, free surface, gelatin, modeling, bullet-jet, shear waves

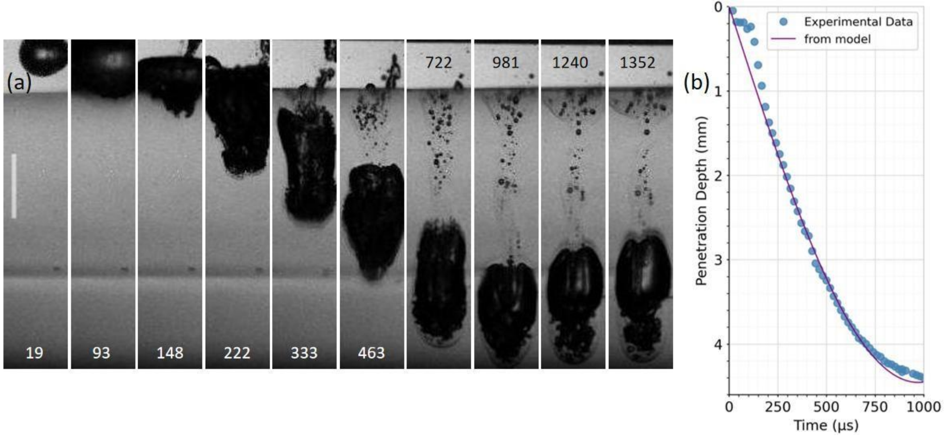

Figure 1. *(a) The bubble collapses and jets into the gelatin. A scale bar representing 1 mm is provided in the first frame. The timing in μs is given in each frame. The bubble expands to its maximum radius of 805 μm at frame t = 93 μs . After which it collapses, jets into the gelatin before retreating upwards. (b) The calculation result from our model is plotted in solid line together with the jet tip positions (blue dots). Initial velocity is taken from experiment to be 7.21 m/s.*

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Effect of surfactants on slide electrification of moving drops

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This presentation is about drops of polar liquid that slide over a hydrophobic solid surface. A typical situation is a water drop sliding down a tilted plate. In recent years it has been realized that such drops spontaneously acquire a charge. The opposite charge is deposited behind the drop as a surface charge. This process is called slide or contact electrification. Slide electrification can generate drop potentials of several kV and substantially influence drop motion. Here we show that the charge of moving water droplets on hydrophobic surfaces is reduced by the addition of surfactant. We attribute the charge reduction to the adsorption of surfactant on the solid surfaces during wetting and the desorption of pre-absorbed surfactant during dewetting. The reduction of charge by surfactant may help to eliminate possible surface corrosion with the disappearance of the high potential formed by sliding electrification.

Keywords: Wetting, Contact angle, Contact electrification, Slide electrification, Surfactant

Prediction of non-linear oscillatory experiments by stress activated EVP models

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Elasto-viscoplastic (EVP) fluids are characterised by both a solid behaviour at small stresses and a strain-rate dependent fluid behaviour at high stresses. Historically, this behaviour is represented by a hard threshold called the static yield-stress, e.g. the Herschley-Bulkley (HB) model [1]. A minimalistic EVP model was recently proposed, which replaces the yield stress by a stress activated shift of the relaxation time [2]. The model assumes the same physical behaviour of the material, both in "solid" and "fluid" state, the relaxation processes being accelerated by the applied stress to show a different phenomenology. This is expressed by a stress-activated plastic viscosity that controls the relaxation of the elastic strains accumulated by the deformation. A concentrated Carbopol 940 dispersion was chosen as representative material of simple-yield stress fluids (i.e. non-tixotropic EVP fluids that exhibit simple plasticity).

The use of Large/Medium oscillatory shear (LAOS/MAOS) has gained a lot of attention recently for the description and modelling of EVP materials [3,4,5,6]. These techniques have the great benefit to probe the non-linear response of a material with an experimentally simple protocol. Moreover, several physical processes are recognizable from the acquired data.

In the present work, we will use MAOS measurements (as the first departure from linearity and solid behaviour) to compare the prediction of the simple shear model [1], its tensorial extension, and various standard models (e.g. HB model). We will demonstrate how the stress activated nonlinearity is reflected in the typical physical interpretation of non-linear oscillatory experiments.

Keywords: EVP material, LAOS, yield-stress, Carbopol, constitutive equations, soft glassy materials

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Quantifying the asymmetric viscoelastic response of dense PNIPAM suspensions subjected to heating and cooling temperature ramps

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We synthesized poly (N-isopropyl acrylamide) (PNIPAM) microgel particles by the free radical precipitation polymerization method using a polar crosslinker. PNIPAM particles in aqueous suspension exhibit thermoresponsive behavior and display a volume phase transition temperature (VPTT) at approximately 33°C. As these particles are deformable and compressible, we determined their average hydrodynamic diameter in dilute solution using dynamic light scattering. We prepared dense aqueous suspensions of PNIPAM microgel particles with a constant effective volume fraction of 1.6 at 25°C. We studied the relaxations of the viscoelastic moduli of these dense suspensions during heating and cooling under various temperature ramp rates below the VPTT. We found an asymmetry in the relaxation of the storage modulus during the heating and cooling processes. This asymmetry, which became increasingly more significant when slower temperature ramps were applied, was quantified as the ratio of the area under the storage modulus-time plot during the heating process to that during cooling. The relaxation response of the loss modulus was characterized by peaks at the times of initiation and termination of the temperature ramp. These two peaks indicate dissipation due to the rearrangement of the colloidal microgel particles in response to sudden temperature changes. Notably, we found an inverse correlation between the asymmetry of the storage modulus and the peaks in the loss modulus. Our results demonstrate that energy dissipation through microgel rearrangements can successfully eliminate asymmetries in the storage modulus of dense metastable PNIPAM suspensions. Finally, we verified the abovementioned inverse correlation by varying the frequencies of oscillation and effective volume fractions of dense suspensions of PNIPAM particles.

Keywords: Microgels, Thermoresponsive, Volume phase transition temperature (VPTT), Asymmetries, Rearrangements

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Bidispersity-driven tuning of mechanical properties in capillary suspension gels

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Capillary suspensions are particulate systems stabilized by networks of liquid bridges formed between particles immersed in two immiscible liquids (Figure 1 A), resulting in gel-like materials with tunable mechanical properties. Incorporating bidisperse particles into capillary suspensions expands the achievable microstructures, offering an approach to engineer composite materials with enhanced mechanical behavior. However, the structural and rheological implications of particle size and concentration disparities in bidisperse capillary suspensions remain largely unexplored.

In this study, we systematically investigated bidisperse capillary suspensions across diverse particle size ratios and concentration fractions. Rheological characterization, complemented by confocal microscopy, enabled the identification of five distinct microstructures. We also determined critical fractions of larger particles that preserve gel-like integrity, even when significant particle size disparities exist. Based on these results, we developed a phase diagram that serves as a practical guide for tuning suspension microstructure and rheological properties.

Numerical simulations using coupled discrete element method (DEM) and computational fluid dynamics (CFD) were consistent with experimental observations, providing deeper insights into the dynamics of microstructure formation and suspension stability. Notably, simulations demonstrated that at high size disparities and elevated fractions of large particles, smaller particles became embedded within liquid bridges (Figure 1 B), significantly enhancing gel strength and elasticity beyond that achievable with solely small particles. Conversely, at low fractions of larger particles, disruption of the gel network occurred, leading to weaker gels with diminished elasticity.

Keywords: Capillary suspensions, Gel, Bidisperse particles, Rheology

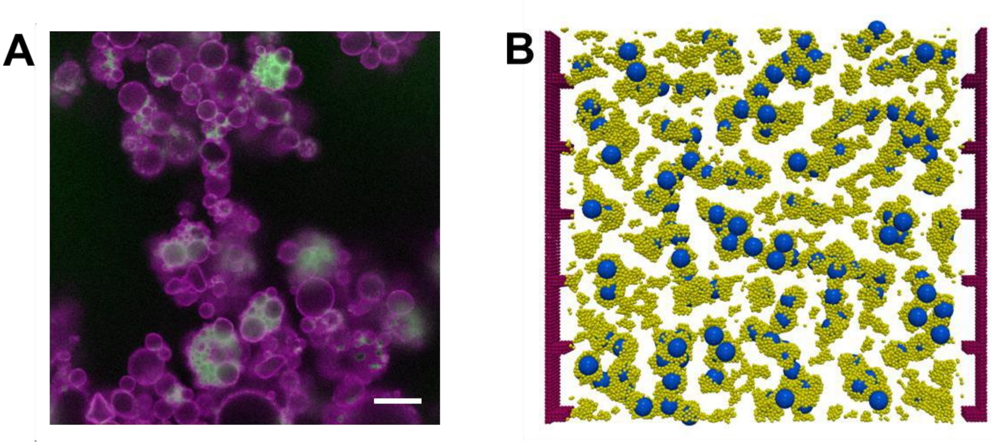

Figure 1. *CLSM image (left) and DEM-CFD numerical simulation (right) of a capillary suspension composed of bidisperse 5-25 μm particles. In the CLSM image, particles are highlighted in magenta, and bridges are dyed green. In the numerical simulation snapshot, small particles are colored yellow, large particles are magenta, and the bulk phase is transparent. Small particles tend to embed in the liquid bridges formed between the large particles.*

Flow or deformation: Timescale competition between medium relaxation time and suspension structuring under oscillatory flow

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The formation of particle strings under shear in viscoelastic media is an elegant method to induce anisotropy in suspensions: Shear thinning and elastic stresses, quantified by the Weissenberg (Wi) number, arise in the medium under flow and drive the particles to arrange in pearl-necklace like string structures [1,2].

While alignment is desired for many applications, such as the formation fibers in biopolymer solutions, or of fibrous meat analogues, the required high shear rates thus elastic forces for viscoelasticity-induced alignment precludes such implementations. By applying oscillatory shear protocols we mitigate this and achieve more feasible processing conditions.

We find that the efficiency of string formation initially increases with fluid elasticity, as opposed to the case for laminar flow in Newtonian media, where reversibility of the flow is retained. Surprisingly the structuring effect decreases for highly elastic systems. At «high» elasticity, particle motion becomes increasingly reversible, and the structuring advantage of oscillatory protocols diminishes. We first perform rheological characterization of various polymer solutions to extract their relaxation spectra. We then conduct particle structuring experiments under oscillatory shear across a range of amplitudes and frequencies. Using optical microscopy coupled with computer vision, we quantify the extent of alignment and correlate it with the underlying rheological timescales. Furthermore, we investigate the length scale over which particles are pulled in by tracking the displacement throughout the structuring process. Finally we track and resolve the ability of the particles to rotate within a string and connect it to the medium elasticity.

This allows us to delineate the regimes (frequency, relaxation time and oscillation amplitude dependent) in which the medium behaves as a viscous, flow-dominated system—enabling irreversible particle displacement between oscillations and string formation—and those in which elastic effects dominate, suppressing net displacement and structure development.

Keywords: Viscoelasticity, Flow-induced assembly, Suspensions, Rheo-optics

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Slip and electrostatics of polyacrylic acid microgels in hydroalcoholic systems

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Carbopol is a brand name for a group of synthetic polymers made from polyacrylic acid (PAA) that are commonly used rheology modifiers in a range of products from distinct industries, including pharmaceuticals, cosmetics, and personal care.

Electrostatics play an important role in Carbopol swelling capacity and on how they can be used in different formulations: Carbopol swells best in high-dielectric constant solvents, where its carboxyl groups ionize and repel each other.

Wall slip can occur in microgels: the sample slides at its interface with a smooth surface due to the presence of a lubricating solvent-only layer. While this is considered a problem in rheology and industry, it can yield interesting insights into the microscopic behaviour of microgels in wateralcohol mixtures.

In this work we investigate how electrostatics influences slip and the rheology of PAA in hydroalcoholic systems. Two Carbopols were tested (974P – hydrophilic, and Ultrez-20 – hydrophobically modified), and water and alcohols with different dielectric constants (Methanol, Ethanol, or Isopropanol) mixed to different compositions were investigated.

Gels made from both Carbopols are found to exhibit slip when the solvent is pure water. However, the way the slip behaviour evolves with increasing alcohol content is different. Transmittance measurements, which are sensitive to the refractive index difference between microgel particles and the solvent, show an increase in turbidity for the hydrophilic Carbopol with increasing alcohol content. However, the transmittance of the hydrophobized Carbopol is nearly solvent independent, indicating that the added alcohol penetrates both microgels differently.

We hypothesize that added alcohol does not significantly penetrate the hydrophilic Carbopol, so that the particle's core display increasing dielectric contrast with the solvent as the alcohol content increase; in contrast, alcohol-water mixtures of different compositions can penetrate hydrophobic Carbopol, giving rise to near-index-matching. We speculate on the relevance of these results for the observed slip behaviour.

Keywords: microgels, polyacrylic acid, rheology, slip, electrostatics

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Rheofluidics: single-drop oscillatory rheology with microfluidics

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The measurement of frequency-dependent viscoelastic moduli is of paramount importance in many fields, from material science to biology, and is typically accomplished in bulk materials using commercial rheometers. The trend towards miniaturization in the biotechnology, manufacturing and chemical processing industries has motivated the extension of viscoelastic measurements to microscopic objects with well-defined shape and size such as droplets, vesicles, microcapsules, or even single cells. For instance, local mechanical probes such as AFM nanoindentation can be used to probe single-cell stiffness, and micropipette aspiration probes the interfacial properties of droplets and vesicles [1,2]. Despite their versatility, these techniques are characterized by complex deformation geometries and a relatively low throughput, which makes them unfit to sample highly heterogeneous populations such as those typical of biological samples. To this end, novel microfluidic approaches have been recently developed to measure the stiffness of cells and droplets flowing through narrow channels. These approaches are well-suited for applications requiring a high throughput, but they lack the fine control of stress and strain required by quantitative mechanical measurements. Here, we present a novel technique called Rheofluidics, which combines the high throughput of microfluidics with the versatility of traditional rheological probes. Like a stresscontrolled rheometer, Rheofluidics measures the time-dependent deformation of droplets subject to a well-defined hydrodynamic stress, whose time evolution is controlled by the shape of the microfluidic channel in which the droplets are flowing. To validate this approach and to demonstrate the power of this technique, we study the linear and nonlinear rheology of oil droplets, hydrogel beads and lipid vesicles, extracting their viscoelastic properties with a throughput more than 1000 times higher than that of standard rheology.

Keywords: rheology, microfluidics, drops, vesicles

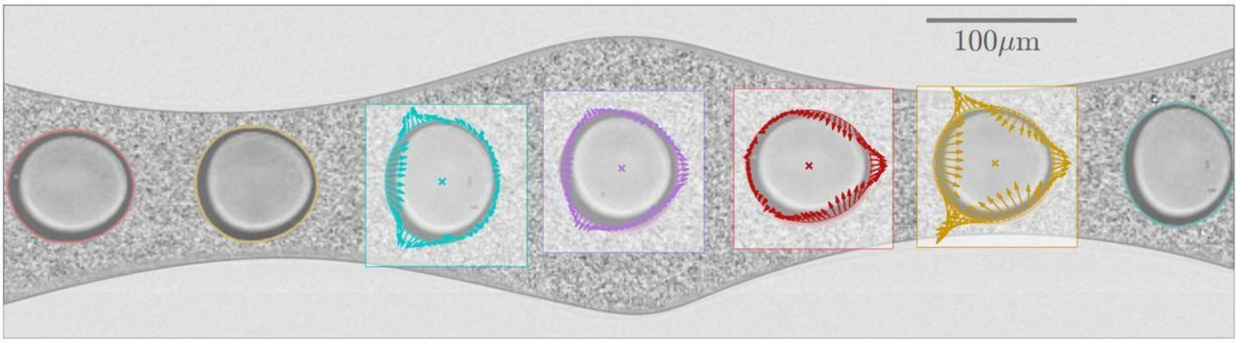

Figure 1. *Reconstruction of a drop flowing through a Rheofluidic channel.*

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Cross-Stream Focusing of Soft Capsules in a Square-Wave Microfluidic Channel

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We present a numerical investigation of the cross-stream migration and focusing behavior of a deformable capsule within a square-wave serpentine microchannel, highlighting the interaction among fluid inertia, capsule deformability, and geometry-induced secondary flows. The capsule is modeled as a fluid-filled elastic membrane and simulated using a coupled lattice Boltzmannimmersed boundary framework [1]. A broad parameter space, with Reynolds numbers up to 360 and a wide range of capillary numbers, is explored to capture both inertial and elasticity-driven effects.

In the wall-normal direction, increasing the Reynolds number promotes outward migration consistent with the Segré-Silberberg effect [2,3], which is progressively weakened by increasing deformability. In the lateral direction, capsule trajectories exhibit a non-monotonic dependence on both inertia and elasticity. At intermediate Reynolds numbers, Dean's drag induced by the channel geometry drives the capsule toward vortex centers, with stiffer capsules showing greater lateral displacement. However, at higher Reynolds numbers, soft capsules no longer focus laterally and remain near the channel centerline—deviating from the nearly capillary-independent focusing observed in smoothly curved geometries [4].

These migration dynamics are governed by a complex interplay among inertial lift, Dean's drag, and deformation-induced resistance to cross-stream transport. The correspondence between capsule focusing positions and the vortex centers extracted from the unperturbed flow field underscores the relevance of secondary flow structures in designing microfluidic devices for deformability-based sorting and separation.

Keywords: Capsule dynamics, inertial microfluidics, Dean's vortices, microfluidic sorting

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Fluid flow in 3-dimensional porous granular systems shows power law scaling with Minkowski functionals –Dependence on particle density

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Understanding flow through porous medium continues to be an active research area because of its important applications in our daily life - from subsurface flow important to agriculture, oil, and natural gas harvesting, CO2 sequestration in sedimentary rocks to engineering applications, fluid transport in the pore space of a granular 3-dimensional structure is a complex non-linear problem. Transport of fluids in real situations, e.g., sedimentary rocks, is characterized by permeability or conductivity. However, these macro properties of the porous system are guided by micro to mesoscale properties like the size and shape of grains, which can have a wide distribution. Our work in this paper is inspired by Hadwiger's characterization theorem, which roughly says that the structure of finite unions of convex subsets of 3- dimensional systems can be described by at most four invariant measures - the Minkowski functionals. Therefore, it is not unreasonable to expect that all transport properties, e.g., permeability, may be linked to the basic invariant geometric measures of the porous medium, as the grains can be assumed to be roughly convex. In this work we explore and develop a relationship between the four suitable Minkowski functionals and pore-scale properties of 3- dimensional systems. We systematically study the dependency of permeability on the geometrical characteristics of 3-dimensional porous systems generated stochastically. Our studies reveal that for 3-dimensional porous system permeability k follows a scaling relation with the four Minkowski functionals: (a) volume of the pore space, (b) integral mean curvature, (c) Euler Characteristic and (d) critical cross-sectional area of the pore space. We explore this dependence with respect to particle density of the system

Keywords: Granular porous media, Fluid transport, Permeability, Micro-property, Power law

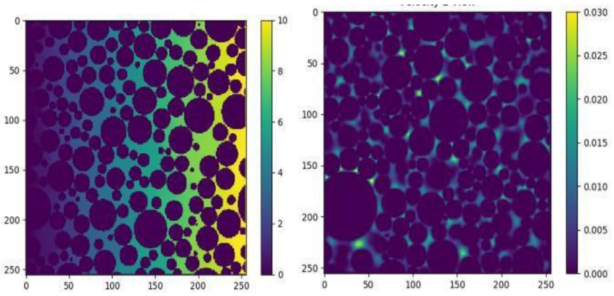

Figure 1. *Velocity field variation with particle density*

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Sequence-programmable and mechanically tunable DNA hydrogels

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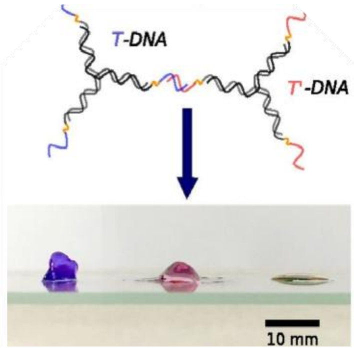
Hydrogels represent three-dimensional porous networks and form due to the ability of a particle or polymer to absorb significant amounts of water. Self-assembly triggered by physical or chemical interactions then continues until the controlled formation of a functional and stimuli-responsive network. Utilising DNA to construct such networks offers significant benefits, e.g. high biocompatibility and unmatched programmability of interactions and mechanical adjustability. DNA hydrogels are temporary self-repairing networks that associate and disassociate reversibly when prompted by external factors, often temperature changes. This characteristic categorises them as physical hydrogels, which hold promise for applications in biosensing, artificial tissue engineering, and data processing, where precision in recognising and binding a target is crucial.

In collaboration with former colleagues from the University of Cambridge and Tsinghua University, we initiated studies on the link between DNA oligonucleotide composition and large-scale mechanical properties of DNA-hydrogel networks. Our publications in *PNAS* [1] (Fig. 1) and *Soft Matter* [2] demonstrate the impact of modifying the composition of 'sticky ends' that connect DNA nanostars or altering the degree of flexibility of the network. Reducing the bases involved in the connection of DNA components decreases the gel network's 'melting point.' In contrast, increasing nonbinding bases or introducing mismatches (point mutations) can weaken the overall structure. Our current objective is to systematically investigate how microstructure and macroproperties are connected by generating a database of DNA-hydrogel networks with customisable mechanical traits. To this end, we plan to use an approach combining both simulations and experiments, integrating oxDNA and LAMMPS modelling with experimental microrheology data. In the near future, we can envisage this empirically informed database to be used in machine-learning algorithms to predict structures formed from individual oligos.



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Tuesday 30th September 2025

C. Colloidal matter

(Room 1)

Demixing and intertwined double networks: a design concept based on network architectures

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Natural and synthetic multi-component gels display emergent properties, which implies that they are more than just the sum of their components. We have developed a new model and computational approach to investigate the effect of changing the strength of the interaction between two species forming a fibrous double network [1]. Simply changing the strength of inter-species lateral association generates two types of gels: one in which the two components demix, and another one in which the two species wrap around each other.

We show that demixing gels have structure and rheology that are largely unaffected by the strength of attraction between the components. In contrast, architecture and material properties of intertwined gels strongly depend on inter-species ``stickiness'' and volume exclusion. These results can be used as the basis of a design principle for double networks which are made to emphasize either stability to perturbations or responsiveness to stimuli. Similar ideas could be used to interpret naturally occurring multi-component gels. Based on these results, we have analyzed how the distinct types of double network architectures determine plasticity and toughness [2].

Keywords: Double networks, self-assembling gels, plasticity, toughness.

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Diffusion and flow in complex fluids

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Brownian motion is fundamental for describing diffusion across a wide range of systems, from simple solvents to highly complex biological and industrial fluids. Unlike simple liquids consisting solely of solvent molecules, complex liquids—such as colloidal suspensions, polymer solutions, or the cellular cytoplasm—contain multiple constituents varying significantly in size and shape. Capturing Brownian dynamics in these multiscale environments poses significant theoretical challenges due to the essential role of direct and many-body hydrodynamic interactions. Traditionally, diffusion theories emphasize particle crowding effects, overlooking that the diffusion dynamics fundamentally depend on the hydrodynamic interactions encoded in the wave-vector-dependent viscosity. Wave-vector- dependent viscosity characterizes the fluid's hydrodynamic response. It describes how viscosity varies with the length scale at which the fluid is probed, capturing complex hydrodynamic interactions across different scales.

This work focuses on the wave-vector-dependent viscosity as the central hydrodynamic quantity. This novel perspective enables systematic investigations of the diffusivity of tracer particles spanning several orders of magnitude in size, providing exact microscopic expressions for both short- and long-time self-diffusion coefficients. We explore Brownian motion from this new perspective, explicitly analyzing diffusion as a function of probe particle size. By studying the limits of small and large particle sizes across various theoretical approximations, we highlight our approach's potential and current limitations. This perspective offers broader applicability and deeper insight into diffusion phenomena, promising advances in understanding and modeling complex fluid environments.

Keywords: diffusion, complex fluids, wave-vector dependent viscosity

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Complex Diffusion of colloidal Tracers within ordered and disordered Arrays of Micropillars

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Despite a wide spectrum of observations, Fickian non-Gaussian Diffusion (FnGD) remains a major open issue in soft matter [1]. However, it is commonly accepted that the emergence of FnGD is related to the presence of some structural or dynamic heterogeneity of the environment [2]. Recent advances in this direction have arisen from the identification of convenient model systems, where the degree of FnGD can be finely tuned by changing some control parameters, and the dynamics can be monitored over broad time windows with sufficient statistics [3]. The results obtained for these systems indicate that FnGD is usually preceded by anomalous diffusion, and the two regimes are closely tangled.

In this work, we consider diffusion of colloidal tracers in a static environment characterized by structural heterogeneity. In particular, structural patterns consist of arrays of micro-pillars realized by mask less photolithography at different degrees of randomness, symmetry, and pillar density. We tracked the motion of particles diffusing in 2D on time scales one order of magnitude longer than the Brownian time [4], greatly extending the time window probed in a previous study of FnGD on similar systems [5].

We compare the experimental results with Brownian Dynamics simulations and identify the characteristic time and length scales that control FnGD in the investigated system [6].

Keywords: 2-D Diffusion, Fickian non-Gaussian Diffusion, Structural heterogeneities

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Impact of surface asperities on shear rheological properties of a particle laden interfac

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Surface heterogeneities in micro- and nanoparticles, whether chemical or topographical, significantly influence self-assembly and interfacial mechanics. At fluid-fluid interfaces, lateral capillary forces with a dominant quadrupolar term arise from undulations in the contact line, which govern particle interactions and the mechanical properties of the spanning network of the particle-laden interface [1].

The impact of topographical features on mechanical properties was investigated through different organo-silica microparticles with comparable diameters and surface chemistries.

We examined the interfacial mechanical properties of these microparticles with convex and concave surface features at a water-air interface. The resulting networks were studied in a Langmuir trough with an adapted double-wall ring (DWR) setup, while optical microscopy was used to track local structural rearrangements and observe the surface coverage of particles at the interface [2].

Optical tweezers were employed to trap particles at an oil-water interface to probe particle-particle interactions, providing insights into force contributions and anisotropies in lateral capillary interactions [3]. These measurements aim to establish a constitutive relationship between surface roughness, particle-particle potential, and interfacial shear rheology. Preliminary results demonstrate a highly elastic and robust interface in the high-frequency regime due to the interlocking of particles with more pronounced asperities. The interlocking of particles could be further enhanced by incorporating complementary convex and concave asperities, utilizing a lock-and-key mechanism against shear deformation.

Keywords: Particle laden interface, lateral capillary forces, optical trapping, Interfacial shear rheology

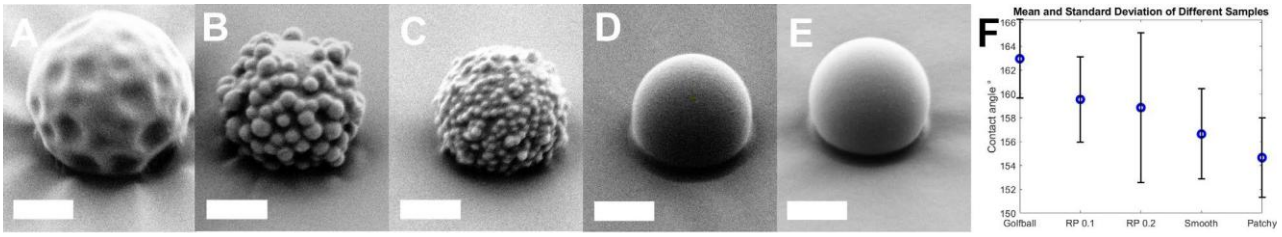

Figure 1. *SEM micrographs taken at a 30° incident angle showing (A–E) microparticles with different surface topographies: concave, convex asperities with 200 nm and 100 nm smaller particles, smooth, and patchy surfaces. Scale bar = 1 µm for all images. (F) Contact angles of 25 particles per class, measured using the gel trapping technique.*

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Experimental investigation of chiral and entropic interactions induced on self- assembly of cellulose nanocrystals (SCNCs)

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Sulfuric-acid hydrolysed cellulose nanocrystals (SCNCs) are highly anisotropic colloidal rods that self-assemble from suspensions into (lyotropic) liquid crystalline (LC) phases as a result of the interplay between different entropic contributions. In these systems, non-isotropic excluded volume interactions among the rods drive their co-alignment and the formation of nematic LC phases above a threshold concentration of about $\varphi^* \sim 3.7$. The cholesteric phase is nucleated by micron-sized nematic droplets, tactoids, formed within the isotropic–nematic coexistence regime.

We experimentally investigated the effect of a chiral environment and the effect of a non- adsorbing natural hydrocolloid (Gum Arabic) on the self-assembly of SCNCs.
In the talk I will describe our experimental observations of 1) Disruption and modification SCNCs assembly in solutions of enantiomerically pure D-alanine solutions. In this system the effect is specific to D-alanine and cannot be attributed to the adsorption of alanine molecules (neither D- nor L-alanine) onto the SCNC particles. 2) The effect of SCNCs crowding induced by non-adsorbing GA hydrocolloids on the phase behaviour and organization of suspended CNCs. The studies were carried out using Transmission Electron Microscopy and cryogenic temperatures (Cryo-TEM), optical microscopy, and Small Angle X-ray Scattering (SAXS).

Circular finger pattern from a slowly drying colloidal droplet

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The drying of colloidal suspensions can be surprisingly complicated. An example is the everyday phenomena known as the "coffee stain effect", where most of the colloidal solid particles are transported towards the rim of a sessile droplet due to hydrodynamic convection currents caused by evaporation [1]. The resulting pattern are generally either uniform, along the rim, form a single or multiple circular rings, or form as a diffusion-limited aggregate [2].

We find that if we throttle the evaporation rate drastically, a different type of pattern will form [3]. Our system undergoes 3 stages of drying dynamics, where the last stage is characterized by a buckling instability that results in a radially symmetric finger pattern (which is also a beautiful labyrinth). The exact mechanism of this instability is still an open question, and we present relevant characteristics and statistics we have obtained in our experiments, both from time-lapse videos and confocal microscopy. Lastly, we present a circular-chord analysis technique we developed to characterise patterns with circular symmetry, which could be used to benchmark a simulation studies and provide information on characteristic length scales in the system.

Keywords: Colloids, Pattern Formation, Drying, Fingering Instability

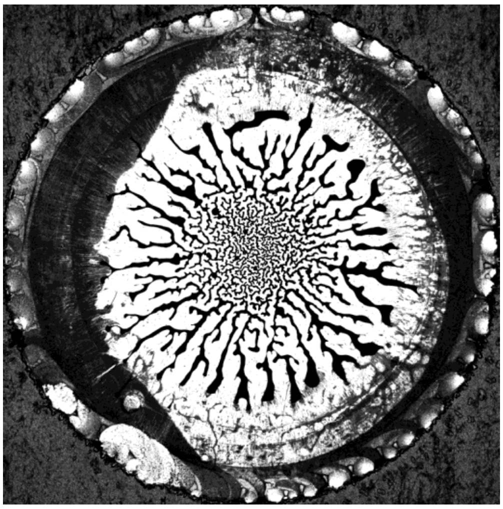

Figure 1. *Example of the patterns resulting from our slow evaporation experiments.*

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DNA mediated colloidal interactions, beyond the simple duplex

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DNA-guided self-assembly of colloidal building blocks has enabled the formation of diverse structures, including clusters, colloidal molecules, polymers, and crystals.[1,2] Leveraging the high selectivity of DNA hybridization, interactions between particles are encoded in short DNA strands that form bridging duplexes at low temperatures. By suspending particles in a tailored buffer, these interactions can be switched ON or OFF by modulating the temperature relative to the system's melting temperature (T_m), which depends on DNA grafting density, sequence composition, and buffer conditions. [3]

In our recent work, we have expanded the DNA toolbox to introduce greater versatility in self-assembly pathways, incorporating light and pH sensitivity as well as responsiveness to free-floating DNA strands. First, by integrating a molecular azobenzene based photoswitch into the sticky ends of DNA grafted onto colloidal particles, we achieve not only ON/OFF switching but also fine-tuned, continuous control of particle interactions using light. An azobenzene moiety undergoes rapid, reversible conformational changes under UV or blue light, modulating DNA duplex stability and, consequently, the system's Tm. This enables precise, localized control of particle aggregation and facilitates isothermal assembly pathways. Second, moving beyond traditional duplex interactions, we explore colloidal self-assembly mediated by DNA triplex formation—supramolecular assemblies involving three strands. The presence of this third strand alters the dynamics of assembly, introduces additional orthogonal control parameters, and enhances the ability of particles to sense their environment. These strategies open new possibilities for programmable colloidal architectures with dynamic and responsive behavior.

Keywords: Self-assembly, DNA brush, intercalant, triplex

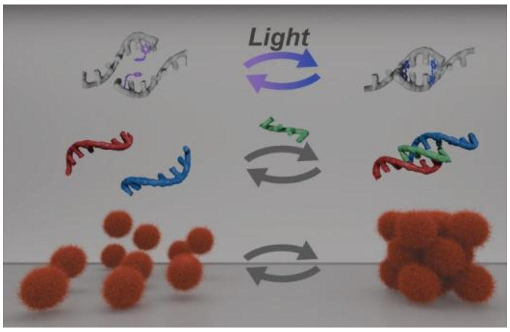

Figure 1. *Extended DNA toolbox for colloidal self-assembly*

Acknowledgements: We acknowledge funding from IdEx Bordeaux (ANR-10-IDEX-03-02), Région Nouvelle-Aquitaine (AAPR 2020-2019-8330510) and from the ANR GOYA (ANR-21-CE06-0016)

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Exploring the phase diagram of soft permeable non-spherical particle suspensions

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The growing demand for enhanced material functionality has recently led to a surge of interest in complex matter systems. Soft colloidal suspensions, in particular, serve as smart building blocks for responsive materials. Their tunable size and capacity to swell and deform in response to various stimuli make them ideal for integration into emerging micro- and nanoscale applications. Although these systems are commonly used in various fields, such as paints, food, cosmetics, and pharmaceuticals, a deeper understanding of them has yet to be fully explored. Specifically, investigating their mechanical behavior numerically remains challenging, as most well-known methods are based on elasticity while neglecting permeability.

Our mesoscale approach to this problem combines both bulk properties at the continuum level and internal particle structure at the particle level using non-equilibrium thermodynamics. Our two-scale dynamic model, which decouples position and shape dynamics—unlike experiments—makes it possible to investigate elasticity and permeability independently [1-2]. Making particular choices for the particle-particle and particle-solvent interactions, we investigate the phase diagram of prolates in quasi-3D space using particle-based simulations. Comparing previously investigated hard spherical [3] and non-spherical [4] colloids reveals the potential of soft permeable colloids in modern applications such as 4D printing.

Keywords: Non-spherical soft colloids, multiscale modelling

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Self-Organization of Magnetic Rod Suspensions in Oscillating Fields

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We investigate the dynamics of assemblies of rod-shaped magnetic colloids under the influence of an external oscillating magnetic field. Using molecular dynamics simulations, we analyze the emergence of self-organized patterns driven by the interaction between the rods and the applied field. By systematically varying key parameters such as the rods' aspect ratio, the strength of the external magnetic field, and its oscillation frequency, we explore the structural and dynamic properties that govern the evolution of these assemblies. The interplay between magnetic interactions, thermal fluctuations, and external field parameters plays a crucial role in determining the emergent structural organization [1-2], highlighting the complex nature of these systems. Our findings contribute to a broader understanding of pattern formation in driven magnetic colloidal systems, with potential implications for controlled self-organization and tunable material design.

Keywords: Magnetic Rods, Molecular Dynamics, Oscillating Fields, Self-Organization.

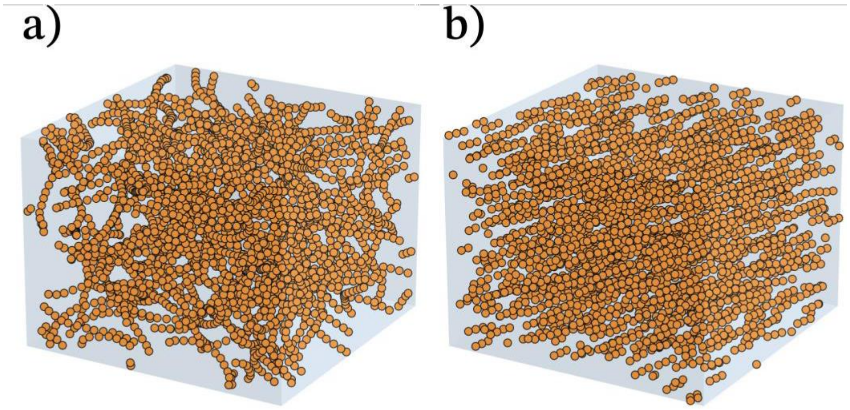

Figure 1. *Pattern formation of magnetic rods under (a) zero magnetic field; (b) an in-plane rotating magnetic field.*

Acknowledgements: The authors acknowledge funding by the European Union under Horizon Europe ERA fellowship project "Pattern Formation in Magnetic Spinners" (Pattspin, No. 101130777).

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Light-responsive amphiphilic polymeric nanoparticles

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Nature possesses a vast amount of materials and systems with the unique ability to reversibly change their structure in response to external stimuli. In particular, responsive conformational control changes play an essential role in protein functioning and signaling. Inspired by this, we aim to achieve conformational control over our protein-mimicking amphiphilic polymeric nanoparticles by incorporating three different photoswitches; Donor-Acceptor Stenhouse Adducts (DASA), Spiropyran (SP) and Aryl Azopyrazolium Ionic photoswitches (AAIP) [1-3]. The nanoparticles comprise a random heterograft polymer containing Jeffamine M1000® or glucose side grafts to ensure water solubility whereas *n*-dodecylamine groups induce polymer collapse and form a water deprived hydrophobic pocket. Using post-polymerization functionalization and click chemistry, we successfully synthesized a series of water-compatible random heterograft polymers with covalently attached photoswitches. As the two isomers of each photoswitch differ in polarity, we aim to study the effect of photoisomerization on the single-chain character and global conformation of the amphiphilic polymeric nanoparticles.

The photoisomerization properties were studied for all systems, with AAIP photoswitches demonstrating superior switching speed and stability of the photostationary states. Subsequent conformational studies revealed that incorporation of the new photo-responsive side-grafts showed the formation of collapsed structures. Further in depth studies on the size, shape and compactness of the amphiphilic polymeric nanoparticles and the influence of photoisomerization hereon are being conducted using small angle x-ray scattering and polarity probes. Finally, preliminary biocompatibility tests demonstrated that minor compositional variations significantly impact cell viability, suggesting an intricate balance between polymeric design, structure and resulting biological effects. Obtaining more insight in the structure-interaction relationship will enhance our fundamental understanding of artificial protein mimics, and allow better design for interaction control in biological applications.

Keywords: Light-responsive, amphiphilic polymers, protein-mimicking nanoparticles

Acknowledgements: We thank the Gravity Program 024.005.020 – Interactive Polymer Materials IPM for funding.

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Dynamics of Particle Assembly in Evaporating Droplets

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When colloidal particles are encapsulated within liquid emulsion droplets, the removal of liquid via evaporation induces self-assembly into distinct packing structures, as illustrated in Figure 1(a). To date, most experimental and theoretical studies are limited to the regime of (i) slow evaporation and (ii) minimal particle friction. In this regime, the final assembly can be predicted through energy minimization and the final packing structure typically minimizes the second moment of the particle distribution. In contrast, here we have coupled lattice Boltzmann and discrete element methods to study the self-assembly process across the full range of evaporation speed and particle friction. We find that the competition between capillary, hydrodynamic, and friction forces can lead to different packing morphologies, see Figures 1(b) and (c). When friction dominates, open packing structures are prevalent. At high evaporation rates but low friction, we find closed but not minimal energy packing. We also examine the influence of initial particle distributions, which allows us to construct a regime diagram alongside probability distributions of the resulting packing configurations. Taken together, our results illustrate possibilities to design the assembly of colloidal particles by fine tuning their dynamical pathway via the liquid evaporation rate and interparticle friction.

Keywords: self-assembly, droplet evaporation, friction, lattice Boltzmann method, discrete element method

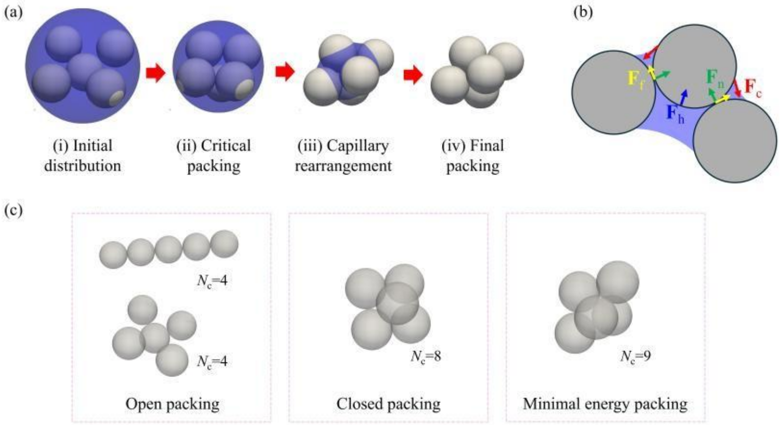

Figure 1. *(a) schematic representation of self-assembly of microspheres via droplet evaporation. (b) The forces applied in the microsphere during self-assembly. F_c is capillary force, F_h hydrodynamic force, F_n contact force, F_f friction. (c) Different final packing schemes considering self-assembly dynamics.*

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Unraveling Molecular Motion in Crowded and Supercooled Aqueous Solutions

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Proteins' movement inside cells and water's behavior under extreme conditions are key to understanding biological function. Here, I present an overview of our recent studies using X-ray free electron lasers (XFELs) to capture crowded protein diffusion and supercooled aqueous solutions.

In a recent study [1], we used X-ray Photon Correlation Spectroscopy (XPCS) measurements at the European XFEL to track ferritin, a model protein, in crowded environments. We found that its motion slows down at high concentrations due to cage effects, where proteins are temporarily trapped by neighbors. A theoretical model based on colloidal theory that includes hydrodynamic and direct protein interactions accurately reproduced our results. These findings are relevant for optimizing drug delivery systems based on ferritin, where diffusion is crucial.

In a related investigation [2], we studied water's unusual behavior at low temperatures using rapid cooling and ultrafast X-ray scattering. We observed an increase in density fluctuations as the system supercooled, reflecting the systems compressibility. Adding glycerol shifted the temperature at which compressibility peaks, linked to water's potential liquid-liquid phase transition. Understanding this behavior can improve cryopreservation methods and other low-temperature technologies.

Keywords: protein dynamics, cage effects, supercooled liquids, x-ray free electron lasers

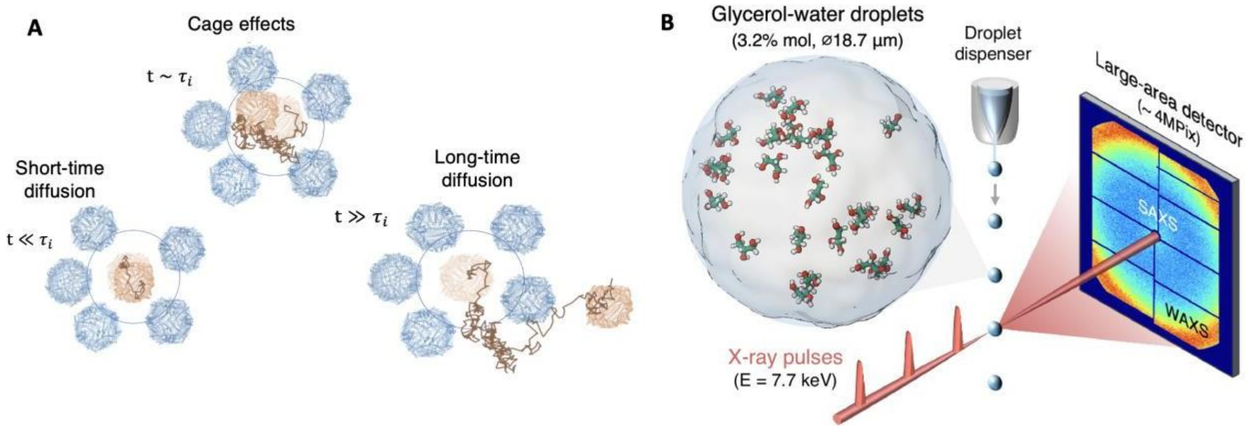

Figure 1. *(A) Conceptual representation of ferritin protein molecular dynamics at different time scales. The panels depict the short-time diffusion (left), cage effects (middle) and long-time diffusion (right) [1]. (B)Schematic overview of the experiment where glycerol-water solution is supercooled by rapid evaporation in vacuum and probed by femtosecond X-ray pulses at SACLA X-ray free-electron laser (XFEL) [2].*

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In situ structural characterization of silica-pNIPAM particles at an air-water interface using contrast variation

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There are various remarkable properties of soft nanogels and microgels such as their thermo-responsiveness once adsorbed to interfaces (i.e. water/air, water/oil) or their use in preparing smart emulsions that can be affected by changes in external stimuli (e.g. temperature and pH-value). When confined at the interface to create responsive emulsions, one of the key parameters determining the droplet stability is the contact angle between the particle and the interface, i.e. where the particle. While there are methods based on microscopy techniques to determine this parameter, they lack the possibility to probe the system in situ and, therefore, how changes in external stimuli affects the structure of the interface. Here, we use neutron reflectometry and contrast variation to characterize the structure of hybrid particle compose by a hard silica core surrounded by a shell of thermoresponsive polymer. The obtained the structural information needed the data are modelled with a costume designed model for core-shell particles at the interface with the aim to better understand the influence of changes in temperature, core size, and shell softness on the structure and position of the particles at the air-water interface. The neutron reflectometry was performed at 20° and 40° Celsius to analyze the differing states of the system under varying temperatures.

Challenging Classical Nucleation Theory: A Rigorous Falsifiability Test

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Classical Nucleation Theory (CNT) is the primary framework for understanding phase transitions, and it is based on the capillarity approximation, which assumes that nucleation properties depend solely on the bulk properties of the melt and crystal phases. However, experiments and simulations have revealed discrepancies between the measured nucleation rates and those predicted by CNT. While these inconsistencies are often addressed through phenomenological adjustments, a fundamental question remains: can this core assumption of CNT be rigorously tested and potentially falsified? To answer this question, we design a falsifiability test [1] that ranks the nucleation abilities of different polymorphs without relying on direct comparisons of nucleation rates, which are often hampered by measurement uncertainties. We create a model system in which all crystal polymorphs share identical bulk and interfacial free energies across all state points. According to CNT, this should result in identical nucleation properties for all polymorphs. Through extensive molecular simulations, we instead observe significant differences in nucleation properties among the polymorphs (see Figure 1), directly contradicting CNT's predictions. CNT fails our test, and this provides strong, clear evidence that the capillarity approximation is flawed: the premise that nucleation is dictated solely by bulk thermodynamics, needs to be reconsidered. Rather than refining empirical corrections, we argue that new approaches to nucleation theory should be developed, approaches that explicitly account for the role of liquid-phase structure.

Keywords: classical nucleation theory, crystallisation, polymorphism, molecular simulations

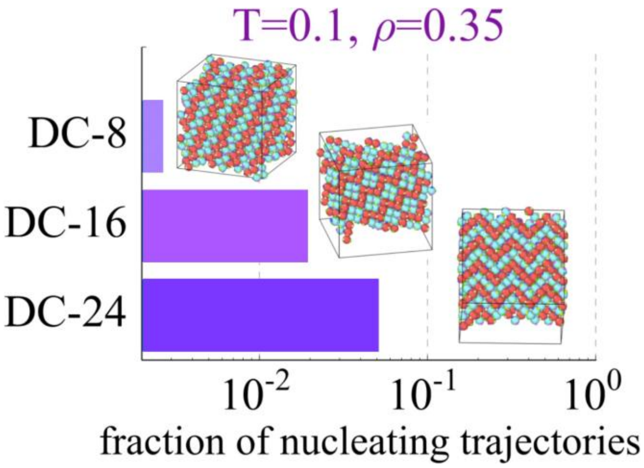

Figure 1. Fraction of nucleating trajectories ending up into each polymorph. *Monte Carlo simulations conducted in the canonical ensemble reveal significant differences in the nucleation behaviours of the three polymorphs. These polymorphs are isotypic forms of the cubic diamond, differing only in the species assigned to the same lattice sites. A snapshot of an extended assembly of each polymorph is superimposed on the histogram.*

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The end of the hard sphere nucleation discrepancy?

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Crystal nucleation is the underlying mechanism of a variety of natural phenomena and technical applications. Consequently, tremendous scientific effort has been devoted to understanding and predicting these fundamental processes over the last few decades. In molecular systems, challenges with an accurate description of the forcefield can hamper accurate predictions [1]. One might imagine that well-controlled, classical model systems would be suitable to address the challenge of predicting the nucleation rate and indeed the most studied material is colloidal hard spheres. Alas, in this system, a discrepancy between prediction and measurement that is so bad it has been termed "the second-worst discrepancy in physics" [2] has persisted for over 20 years (Fig 1a).

Here we provide compelling evidence of agreement between experiment and computer simulation in the nucleation barrier (Fig. 1b). Our results are based on two innovations. Firstly, we consider the start of the nucleation barrier calculated from the size distribution of *pre-critical* nuclei. Secondly, advances in particle-tracking and structural analysis methods enabled us to map our results to hard sphere simulations with hitherto unprecedented precision [3].

But how did the discrepancy come to be in the first place? Measurements of the nucleation rate J appear robust [2], but what about the volume fraction ϕ? Previously, the volume fraction was determined based on the phase behaviour of sedimenting samples, using the method of Ref. [4]. We investigated sedimenting systems with multiscale confocal microscopy (Fig. 1d) and found crystals in the liquid above the liquid-crystal interface (Fig. 1e/f). This leads to a shift in the calculated volume fraction and the origin of the discrepancy.

Keywords: Colloidal Hard Spheres, Confocal Microscopy, Nucleation, Crystallisation

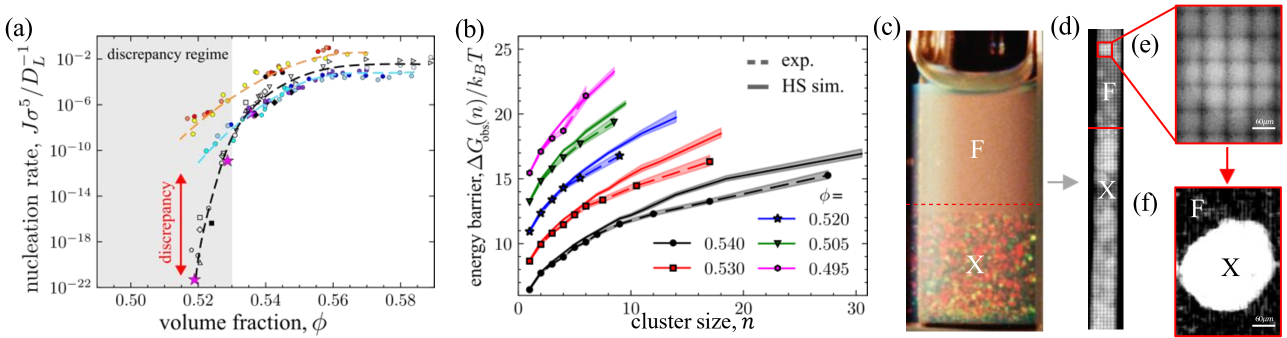

Figure 1. *(a) Reduced nucleation rates J, as a function of volume fraction ϕ, comparing light scattering experiments (coloured) [2] with computer simulations (black) [2] and our data (pink stars) [3]. (b) Nucleation barriers ΔG for computer simulations (solid lines) and experiments (dashed lines) [3]. In (b), data are offset for clarity. (c) Interface between crystal (X) and fluid (F) in sedimenting colloidal hard sphere system [5]. (d) Multiscale confocal image of liquid-crystal interface in a sedimenting sample with $\phi \approx 0.50$. (e) Big crystal in sedimenting liquid above crystal interface. (f) Binary image of crystal in liquid after applying crystal identification algorithm.*

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Self-assembled porous media from particle-stabilized emulsions and evaporation-driven assembly of colloidal films

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We propose a mechanism to create self-assembled porous media with highly tunable geometrical properties and permeabilities [1,2,3]: We allow a particle-stabilized emulsion to form from a mixture of two fluids and colloidal particles. Then, either one fluid phase or the particle layer is solidified, which can be achieved by techniques such as polymerization or freezing. Based on computer simulations we demonstrate that modifying only the particle wettability or concentration results in porous structures with a wide range of pore sizes and a permeability that can be varied by several orders of magnitude. We then discuss the optimization of these properties for self-assembled catalyst support materials and conclude that structures based on so-called "bijels" are the most suitable candidates allowing for an almost threefold increase in reactor effectiveness.

The second part of the presentation focuses on particle self-assembly in drying colloidal suspensions on a solid substrate [4,5]. We numerically investigate the influence of substrate and particle wettability on the deposited pattern. Higher substrate wettability results in a monolayer with a hexagonal arrangement of deposited particles on the substrate. Conversely, lower substrate wettability leads to droplet formation after the film ruptures and, subsequently, particle clusters. Furthermore, we reveal that higher particle wettability can mitigate the impact of substrate wettability and facilitate the formation of highly ordered monolayers. We propose theoretical models predicting the surface coverage fraction dependent on particle volume fraction, initial film thickness, particle radius, as well as substrate and particle wettability, and validate these models with simulations. Our findings provide valuable insights for optimizing the deposition process in the creation of assembled monolayers of colloidal particles.

Keywords: self-assembly, particles at interfaces, drying, lattice Boltzmann simulations

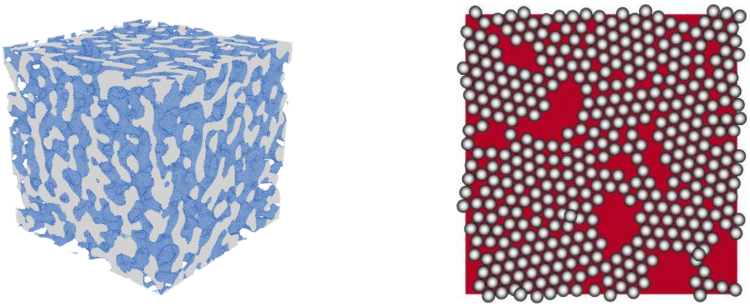

Figure 1. *Left: Porous materials can be obtained from particle-stabilized emulsions. Right: Capillary interactions and particle properties determine the structure of colloidal layers when the solvent evaporates.*

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Dynamic Magnetic Response of Multicore Magnetic Nanoparticles: Influence of Shape Anisotropy

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Over the past few years, multicore magnetic nanoparticles (MMNPs) have drawn considerable interest due to their potential application in various biomedical fields, including targeted drug delivery, magnetic hyperthermia, and biosensors. These nanoparticles consist of dense aggregates of single-domain magnetic nanocrystals embedded in a non-magnetic matrix. Although individual cores typically measure approximately 10 nm, the overall size of MMNPs ranges from tens to hundreds of nanometers. Despite their promise, a thorough understanding of the mechanisms controlling MMNP behavior remains incomplete [1].

In this study, we examine the magnetic properties of multicore magnetic nanoparticles using Brownian dynamics simulations in conjunction with the Landau-Lifshitz-Gilbert equation. All calculations were performed using software package ESPResSo 4.2 [2]. Besides the two types of spherical MMNPs we examined earlier [3], we also investigated MMNPs where the aggregate of single-domain particles had an elongated ellipsoidal shape with a predefined ratio of semi-axes. We calculated zero-field dynamic susceptibility spectra and the orientation distributions of core dipoles relative to their respective easy axes, affected by anisotropy and intercore magnetic interaction strengths. Additionally we evaluated static susceptibilities and performed calculations of the specific loss power. We demonstrate how strongly shape anisotropy affects the dynamic response of multicore particles. Our findings offer valuable insights in advancing applications like magnetic hyperthermia, data storage, and targeted drug delivery using both passive and functionalized active magnetic colloids, where precise control of magnetic dynamics is crucial.

Keywords: magnetic multicore nanoparticles, shape anisotropy, dynamic magnetic susceptibility, magnetic anisotropy, specific loss power, brownian dynamics

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Controlling curvature of self-assembling surfaces via patchy particle design

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Curved structures are ubiquitous both in soft matter as well as in biological and biologically inspired systems. Often, they emerge as a result of self-assembly processes where building blocks aggregate in a controlled manner, giving rise to specific system structure and properties, beyond what is attainable in Euclidean spaces. However, achieving precise control of curvature in assembled structures remains challenging and requires precise control over particle interactions. We introduce an inverse design approach to target self-assembly into surfaces with a specified Gaussian curvature in systems of model patchy particles which are commonly used as a playground to study self-assembly phenomena. Our framework is based on automatic differentiation which enables us to determine parameter gradients by differentiating through the self-assembly kinetics as well as consider arbitrarily complex loss functions. We show how to mitigate the problem of exploding gradients when differentiating over chaotic molecular dynamics trajectories and obtain stable gradients that can be leveraged in general optimization schemes. We outline the model requirements and hyperparameter choices for successful optimization and show that the information gathered from a small number of assembly trajectories is sufficient to yield generalizable optimized potentials. Finally, we demonstrate that the proposed approach allows us to design interactions for self-assembly into structures with a tunable target curvature, paving the way for new functional materials with precisely controlled geometries.

Keywords: self-assembly, curvature, inverse design, differentiable simulations

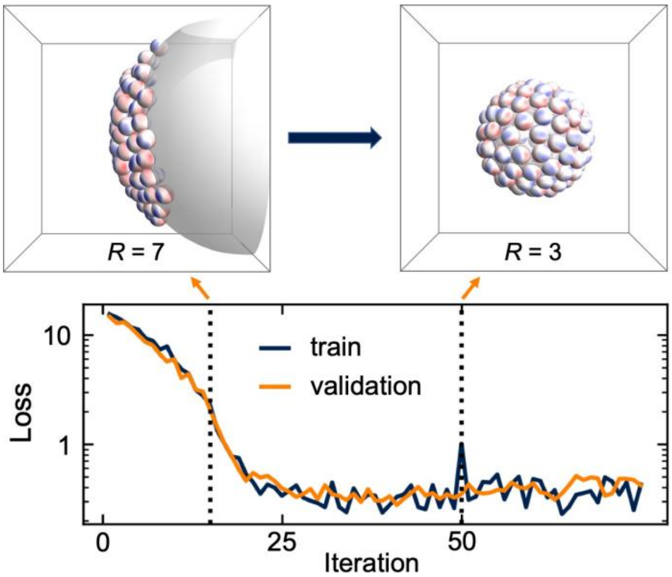

Figure 1. *Optimization of patchy particle interactions for self-assembly of clusters with target curvature.*

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Tuesday 30th September 2025

B. Biological and living matter

(Room 2)

Invasion of bacteria in complex fluids and environments

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Bacteria have the remarkable ability to swim upstream, especially in non-Newtonian fluids [1,2]. This motion against flows can cause not only respiratory, gastrointestinal, and urinary tract infections, but also the contamination of medical devices and hospital equipment. However, it remains unknown how bacteria navigate upstream through these microstructured environments with narrow channels and wide cavities. Here, combining microbiology experiments with nanofabrication and mathematical modeling, we reveal how Escherichia coli invade in four stages: The (I) break-out from colonized cavities against the current, (II) propagation upstream in narrow connectors, (III) infiltration of new cavities, and (IV) colonization with biofilms under flow. Surprisingly, we find that wider channels with faster counterflows are actually more prone to invasion, but these incursions can be inhibited effectively with sharp corner designs. Next, we explore the serial invasion of multiple cavities in a row. We discover that instead of colonizing these nodes one by one slowly, the bacteria rapidly swim all the way upstream and form biofilm streamers there to take possession of the entire channel three times faster. These results shed new light on pathogen motility in host-relevant shear regimes, and they offer solutions that can be implemented directly in biomedical devices.

Keywords: Bacteria, Complex Fluids, Flow Networks, Navigation, Rheotaxis

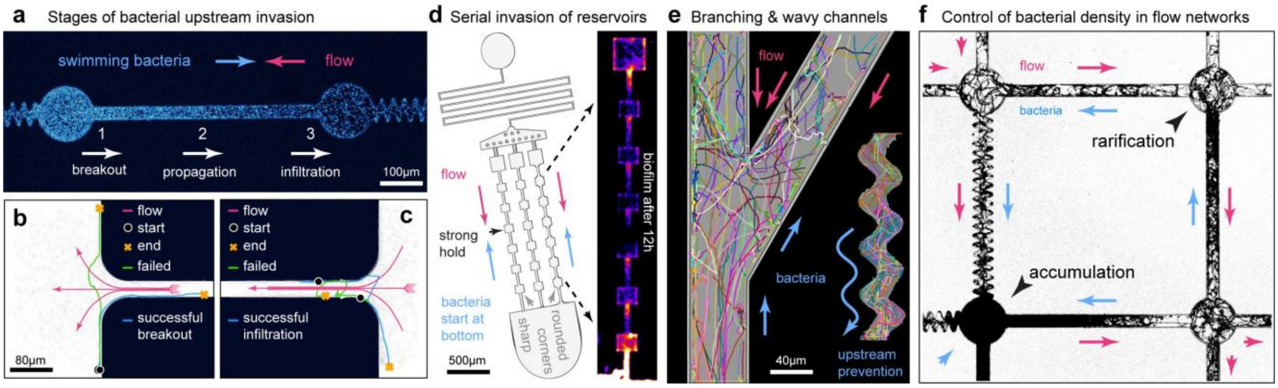

Figure 1. *Invasion of flow networks. (a) Stages of bacterial invasion: Breakout from a colonized cavity, propagation upstream, and infiltration of a new cavity. (b-c) Trajectories of successful break-out and infiltration events. (d) Serial invasion of multiple cavities in a row. Inset: Resulting biofilm formation after 12 hours. (e) Invasion of branching microchannels. Inset: Prevention of upstream migration with wavy channels. (f) Flow networks.*

Acknowledgments: We thank funding from the Charles E. Kaufman Foundation.

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Non-universality of Jamming in Cellular Monolayers

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Phase transitions and collective motion in cellular collectives are central to diverse biological processes, from morphogenesis to wound healing. In particular, the transition from a fluid-like to a solid-like state—often referred to as jamming—has been likened to a glass transition and associated with increasing cell density [1]. However, more recent evidence suggests that other factors, such as cell–cell and cell–substrate adhesion, may play a dominant role [2].

In this study, we critically examine the universality of jamming behavior across monolayers of different epithelial and fibroblast cell lines. By combining Particle Image Velocimetry (PIV) and Differential Dynamic Microscopy (DDM) we find that although all investigated systems display initial ballistic-like motility, their dynamical trajectories toward arrest vary significantly. Some monolayers gradually slow down without changing their motion type, whereas others exhibit a distinct transition from ballistic to diffusive behavior. Crucially, these differences arise not only between epithelial and mesenchymal cell types, but also among cell lines of the same type—demonstrating that jamming is not a universal process governed by a single set of physical rules. We further show that transitions in motility often correlate with the emergence of spatial order within the tissue, reflected in changes in the static structure factor. DDM proves particularly powerful in detecting these signatures, offering reliable access to multi-scale dynamics even under conditions of high density or low contrast.

Together, our findings challenge the notion of universality in the jamming of cellular monolayers and underscore the need for cell-type-specific frameworks to understand collective arrest in living tissues.

Keywords: jamming transition, collective cell dynamics, differential dynamic microscopy

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A Monte Carlo Approach to Simulating Cell Dynamics and Cancer Development

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Understanding how cells behave over time—how they grow, die, accumulate damage, and occasionally transform into cancer cells—is essential for cancer and radiotherapy research. The inherent complexity and randomness of these processes require investigation using simulations and experiments. Cells and tissues can be viewed as a physical complex system, where numerous interacting components give rise to unpredictable behaviors. To better explore these dynamics, a computational approach is needed to complement experimental work and provide insights into long-term tissue behavior.

We developed a computational model that simulates cellular dynamics using Monte Carlo methods [1]. This effort is part of a broader modeling of complex systems, where emergent behavior is studied through the interaction of simple, probabilistically defined rules. The model represents a population of individual cells governed by probabilistic rules for division, death, damage accumulation, and transformation (such as mutations or carcinogenesis). Radiation is introduced as an external factor, and both natural behavior and external influences are treated as stochastic processes evolving over time. The framework includes mechanisms that account for intercellular interactions [2] and history-dependent sensitivity, allowing for a more biologically informed simulation of tissue behavior. These features help capture the variability and complexity observed in real cellular systems.

Through repeated simulations of various conditions, the model illustrates how different scenarios can lead to diverse outcomes, even under similar starting parameters. This variability underscores the importance of stochastic processes in tissue behavior and cancer development.

The model provides a flexible, virtual platform for exploring how different conditions influence long-term outcomes. It can support research into treatment planning, biological mechanisms underlying disease progression, and the impact of various interventions, helping generate hypotheses and refine experimental focus.

Keywords: Monte Carlo simulation, bystander effect, complex system, radiation, cell transformation

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Emergent Mechanics of a networked multivalent protein condensate

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Protein condensates are phase-separated membraneless organelles in living cells. Recent studies have demonstrated that simple one- or two-component protein condensates behave as Maxwell fluids. However, as protein interactions become more complex and the number of protein components increases, the condensates exhibit novel mechanical behaviors beyond Maxwell fluids. The mechanical profiling of multivalent and multi-component protein condensates remains largely unexplored. Here, we characterize the mechanical properties of a functional multivalent protein condensate reconstituted with six postsynaptic density proteins (6xPSD), using atomic-force-microscopy-based mesoscale rheology and quantitative fluorescence experiments. The 6xPSD proteins phase separate into condensate droplets via multivalent protein interactions and oligomerization upon mixing. A key finding of our investigation is that most (80%) of the 6xPSD proteins are mobile and diffuse in a dynamically crosslinked network made of the remaining (20%) non-mobile scaffold proteins. This unique percolating structure gives rise to a two-mode relaxation modulus $E(t)$, featuring an exponential decay at short times followed by a power-law decay at long times. The measured power-law rheology with an exponent of approximately 0.5 marks the binding/unbinding dynamics of the weak bonds in the protein network, allowing the network to rearrange at long times. The simultaneous molecular and mechanical characterizations of the 6xPSD condensate thus provide a reliable platform to investigate the mechanics of functional multivalent protein condensates and their relations to physiological functions and diseases.

Keywords: Protein condensates, Mechanics, Relaxation Modulus, Network, Power law rheology

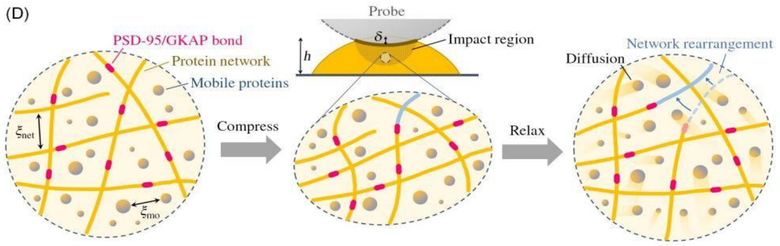

Figure. *Schematic diagrams showing how the 6xPSD condensate under compression relaxes mechanically.*

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The Effects of Electric Fields on Protein Phase Behavior and Protein Crystallization Kinetics

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We studied the effects of an externally applied alternating current (AC) electric field on protein crystallization, liquid–liquid phase separation (LLPS), and crystallization kinetics [1]. Our experiments, summarized in the figure, show that a weak AC electric field significantly alters the location of phase boundaries and crystallization kinetics of lysozyme in the presence of thiocyanate as a precipitant. As seen in the left panel, the crystallization region expands under the electric field, allowing crystals to form within a broader range of conditions, while LLPS is suppressed, reducing the likelihood of a two-step crystallization pathway. The right panel demonstrates that the electric field accelerates nucleation, decreasing induction times and enhancing crystal growth rates compared to the no-field condition. These effects are attributed to modifications in the protein–protein interaction potential induced by the applied field, as illustrated in the schematic inset. Our findings highlight the potential of electric fields as a tool for controlling protein phase behavior and crystallization in various applications.

Keywords: Protein Crystallization, Liquid–Liquid Phase Separation (LLPS), Alternating Current (AC) Electric Field, Nucleation Kinetics, Crystal Growth Rate, Protein–Protein Interactions

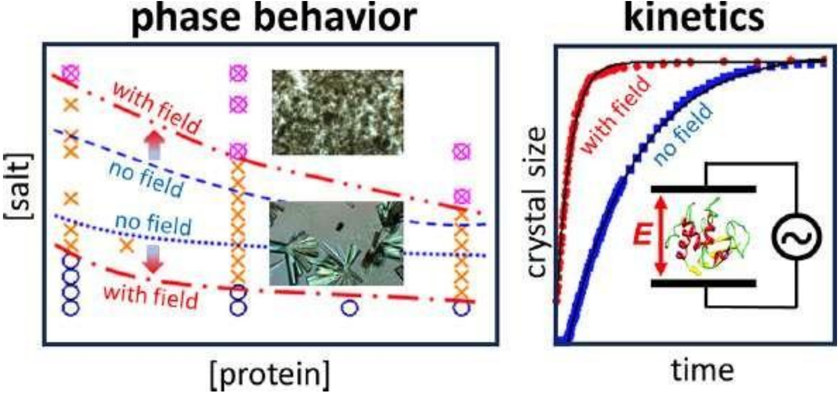

Figure 1. *Effect of an externally applied AC electric field on protein phase behavior and crystallization kinetics. The left panel shows phase diagrams with and without an electric field, demonstrating the suppression of LLPS and the expansion of the crystallization region. The right panel illustrates enhanced nucleation and growth in the presence of the electric field, as indicated by the earlier onset of the growth and steeper increase in crystal size over time. The inset shows a cartoon of a protein exposed to an AC electric field.*

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The dark side of the Moon: biomolecular condensates from the perspective of nucleic acids

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Liquid-Liquid Phase Separation (LLPS) is being increasingly recognized as a relevant mechanism of functional co-assembly of biomolecules in cells, where proteins and nucleic acids (NA) interact in concentrated droplets, which can act as microreactors and catalytic centers [1]. To date, most of the research on such biomolecular condensates has been characterized by a protein-centric perspective, whereas only few studies have focused on NA, often with contrasting results [2,3,4].

We describe here two lines of research which shed some light on the key role of NA properties in regulating LLPS:

i. At the very origin of current biology, the emergence of ribosome stands as one of the milestones of the complex history of protein-NA interactions [5]. We find that, in a wide range of conditions, RNA strands corresponding to minimal versions of the ribosomal core undergo LLPS when mixed with ribosomal peptides [6]. Such compartmentalization into liquid droplets, which protects RNA from degradation, is finely tuned by RNA sequence and structure, and it may have preceded the onset of more specific RNA-protein interactions crucial for the ribosomal activity and structural integrity.

ii. We systematically investigate the LLPS behavior in mixtures of peptides with DNA oligomers of different length, sequence and secondary structure. The main features of the experimental phase diagrams, in terms of temperature and ionic strength, are captured by molecular dynamics simulations based on a chemically specific coarse-grained model. We find that the LLPS propensity of diverse systems is fully determined by NA flexbility and heterogeneity of electrostatic interactions. Moreover, simulations provide insights into structural and dynamic properties of condensates, accounting for the higher observed mobility of peptides.

Keywords: liquid-liquid phase separation, ribosome, secondary structure, coarse-grained model, molecular dynamics simulations

Acknowledgements: We gratefully acknowledge support from 4EU+ European University Alliance.

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Forces and symmetry breaking of a living meso-swimmer

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Swimming is used by a myriad of different organisms spanning micro- to macroscopic sizes. The physics behind swimming at the viscosity-dominated microscale and inertia-dominated macroscale is well studied (**Fig. 1A**). However, in between lies a notoriously complicated mesoscale with swimmers affected by non-linear and time-dependent fluid mechanics. The intricate motility strategies as well as the complex and periodically changing shapes of these meso-organisms add extra challenges for accurately modelling their dynamics. Here, we have further developed the micropipette force sensor to experimentally study the physics of biological meso-swimming dynamics (**Fig. 1B**). We directly probe the swimming forces of the meso-organism *Artemia sp.* and determine how the propulsive force scales with body size [1]. We show that this scaling law is universal for a wide range of micro- to meso-organisms, regardless of body shape, swimming strategy, or the addition of inertia at the mesoscale. Through deep neural network-based image analysis, we determine the time-reversal symmetry breaking of *Artemia* as it transitions from the viscous regime to the mesoscale. We discover that this model meso-swimmer achieves an increased propulsive force by increasing its level of time-reversal symmetry breaking. These results capture fundamental aspects of biological meso-swimming dynamics and provide guidance for future biomimicking meso-robot designs.

Keywords: meso-swimming, propulsive forces, time-reversal symmetry breaking

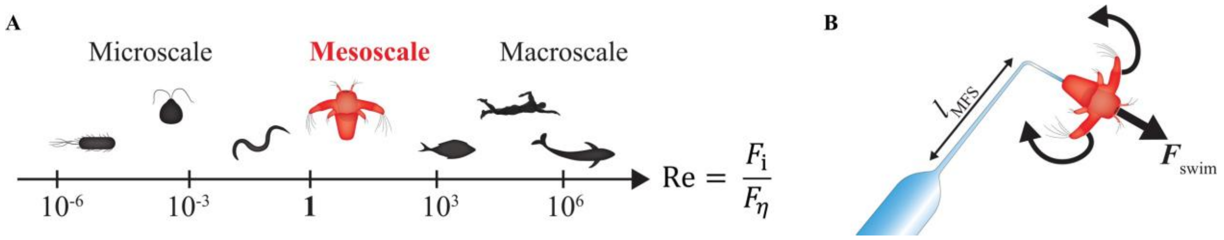

Figure 1. A) *The Reynolds number of organisms with different length scales. The physics behind swimming is well understood at the micro- and macroscale. In the intermediate mesoscale, Artemia (red) has evolved to achieve propulsion in a complicated fluid mechanics regime governed by non-linearities and time-dependencies.* ***B)*** *We have used the micropipette forcer sensor to directly measure the butterfly-swimming dynamics of Artemia.*

Acknowledgements: This work was funded by the European Research Council Starting Grant SWARM and the Research Council of Finland Fellowship MesoSwim.

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Motor-Protein-Driven Intracellular Transport: An Example of Glassy Dynamics?

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While diffusion is sufficient to transport molecules short distances, it becomes increasingly inefficient to transport larger objects longer distances. Transport inside living (mammalian) cells has consequently evolved to take advantage of motor proteins that carry larger objects down the "intracellular highways" constituted by the cytoskeleton. Using live-cell microscopy we have followed beads [1], lysosomes [2], and mitochondria [2] as they are transported by motor proteins in several different mammalian cell types. We observe that, despite the existence of motor-proteins, organelles often remain stationary for extended periods of time before moving larger distances. While this would appear to be an inefficient mode of transport, it looks surprisingly similar to how objects move within a glass. Testing several different hallmarks of glassy dynamics, we find that motor-protein-driven transport in mammalian cells indeed exhibit characteristics of glassy dynamics, thereby providing a different perspective on intracellular motion.

Keywords: glassy dynamics; living cell; motor proteins

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Engineered bacterial cell-cell adhesion for down-stream separation

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Lynne Regan[1]*, Gavin Melaugh*[2]

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We seek to create user-specified associations of bacteria. Engineered microbial communities, have an abundance of potential applications including understanding natural biofilm formation, creating complex living materials and performing metabolic transformations. Controllable, user-specified cell-cell adherence is key to obtaining such associations. Our method is based on the surface display of either SpyCatcher proteins or SpyTag peptides on E. coli. SpyCatcher and SpyTag spontaneously associate, forming a covalent bond [1] and thus, when displayed on the surface of cells, can cause cellular aggregation. We refer to these proteins as CLASPs (Cell Linking Adhesive Surface Proteins). In initial studies we have characterised the way in which this system behaves and can be manipulated. I will present these data. I will also present a potential practical application of this work - enhanced separation of cells by settling in applications such as protein production. This enhanced separation relies on aggregated CLASP cells settling faster than non-adhered cells. Thus, lower centrifugal forces achieve equivalent clearing of the supernatant as higher centrifugal forces with un-associated cells. In this context we will show how CLASP cells can be compatible with more energy efficient protein production due to the reduced time and energy needed for centrifugation.

Key words: Bacteria, Cellular adhesion, sedimentation, synthetic biology

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Rules for chromosome segregation in spherical cells

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In all living organisms, the ability to faithfully replicate the genetic material and successfully distribute it to the two daughter cells is a fundamental condition for the existence of life. For this to succeed, chromosome copies must be correctly separated and positioned at opposite poles of the mother cell before division. This process is known as *chromosome segregation*. In eukaryotes, like animals and plants, chromosome segregation is a tightly coreographed process, which culminates with a microtubules structure -the spindle- mechanically pulling each chromosome copy to a different cell pole.

In prokaryotes, like bacteria and archaea, chromosome segregation is less understood. Despite several segregation machineries having been characterized in bacterial species, very few general principles have emerged. Twenty years ago, it was proposed that one of the main driving forces for prokaryotic chromosome segregation could be entropy[1]: chromosomes are polymers, and when two polymers overlap entropy increases, resulting in an effective force pushing them apart. This mechanism is particularly effective in cylindrical cells, where the shape of confinement breaks the symmetry, directing the entropic force. However, many prokaryotes have spherical cells, suggesting that other mechanisms must be at play.

Here, we develop a minimal coarse-grained model of chromosome segregation in spherical cells (Fig 1), inspired by the experimental study of an archaeon[2]. Our simulations reveal that, while entropic forces contribute to segregation in spherical confinement, they are insufficient on their own for robust separation. To achieve this, a combination of fast compaction of the genome and membrane-chromosome association is necessary. Finally, we show that cell division, by causing the cell to temporarily become more elongated, can mechanically aid segregation. Our work sheds light on the physical principles that enable chromosome segregation in spherical cells and contributes to a deeper understanding of prokaryotic cell division.

Keywords: chromosome organization, polymer physics, entropy, coarse-grained simulations

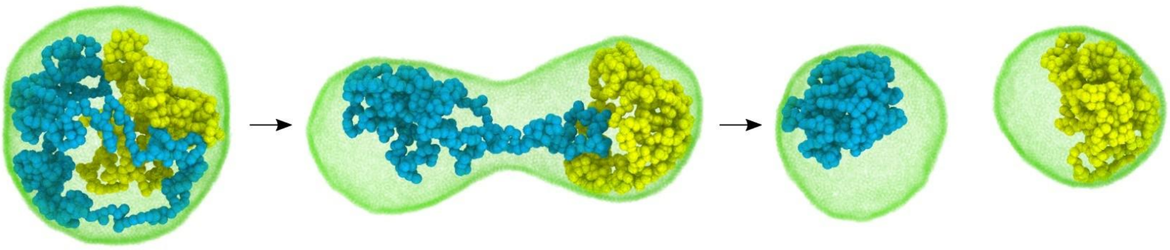

Figure 1. *Molecular dynamics simulations of chromosome segregation and division in a spherical cell. The two chromosomes, modeled as ring polymers, are colored blue and yellow, respectively, while the cell membrane is green.*

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A multiscale coarse-graining approach for the description of charge effects in antibody solutions

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Colloidal models are commonly used to describe protein-protein interactions and their effects on solution properties. However, proteins are much more complex than the typical hard sphere-like synthetic model colloids. This is particularly true for monoclonal antibodies [mAbs], where the anisotropic Y-shaped structure combined with a complex and heterogeneous charge distribution requires much more refined models. Here, we report the results of a systematic investigation of the solution properties of charged IgG1 mAbs as a function of concentration and ionic strength using a combination of electrophoretic measurements, static and dynamic light scattering, small-angle x-ray scattering (SAXS), and tracer particle-based microrheology [1,2]. We analyse and interpret the experimental results using established colloid theory and coarse-grained computer simulations. Particular attention is given to the role of charges and their distribution on the antibody surface. These charges not only strongly influence solution properties, the colloidal stability and the phase behavior of the mAbs, but need to be taken into account during the preparation of high concentration samples through ultrafiltration using centrifugal concentrators. Here the Gibbs-Donnan effect results in a concentration-dependent final pH and ionic strength that in turn changes the charge state and the electrostatic contribution to the protein interactions. Using a multi-scale coarse graining strategy that starts from the known molecular structure of the protein, we develop models based on analogies to soft particles such as star polyelectrolytes. We demonstrate that our approach is able to reproduce and predict the concentration dependence of the structure and dynamics of antibody solutions over a large range of length and time scales, concentrations and ionic strengths.

Keywords: coarse-graining, antibody solutions, light and x-ray scattering

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Interaction of the Parkinson's-Related Intrinsically Disordered Protein α-Synuclein with Differently Charged Biomembranes

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Intrinsically disordered proteins (IDPs) lack a defined three-dimensional structure but can adopt specific conformations upon interaction with binding partners. α-Synuclein (α-Syn), a neuronal IDP, is closely associated with neurodegenerative disorders such as Parkinson's disease, where its aggregation into fibrils plays a key pathological role [1]. α-Syn's interaction with lipid membranes is a critical factor influencing its aggregation, toxicity, and contribution to disease progression [2]. However, the molecular mechanisms underlying these interactions remain poorly understood.

Neutron Reflectometry (NR) was employed to investigate the interaction of α-Syn with supported lipid bilayers of varying charge compositions. The bilayers, composed of partially deuterated DMPC and DMPG lipids, were analyzed to assess structural changes upon protein binding. Circular Dichroism (CD) and Infrared (IR) spectroscopy were used as complementary techniques to examine secondary structure formation and membrane changes during protein-membrane interactions.

NR revealed that membrane charge plays a crucial role in α-Syn binding and its ability to disrupt membranes, showing detergent-like behavior. The binding interactions were relatively weak, maintaining an equilibrium between free and membrane-bound proteins. Temperature-dependent effects were observed, with distinct behaviors at different temperatures. CD spectroscopy demonstrated a formation of α-helical structure upon binding to charged membranes, while IR spectroscopy confirmed α-Syn's detergent-like activity and its ability to destabilize membrane integrity.

This work addresses critical gaps in understanding α-Syn's interactions with membranes and its associated toxicity. It emphasizes the importance of membrane charge, pre-existing damage, and temperature in modulating α-Syn behavior. These findings enhance our understanding of α-Syn's role in neurodegenerative disorders and provide valuable insights for identifying potential therapeutic targets to mitigate its pathological effects.

Keywords: alpha-Synuclein, Intrinsically Disorder Proteins, Neutron Reflectometry, Phospholipids membrane, Parkinson disease

Acknowledgements: D17 beam time at ILL, CD DISCO Spectroscopy beam time at SOLEIL

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Quantifying Flexible Defect Excitation in Sharply Bent DNA

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DNA is a stiff polymer with a persistence length of around 50 nm. DNA sharp bending below the length scale of 50 nm should cost huge energies but occur in many biological processes. To obtain DNA sharp bending energies, many experiments were designed and the results suggest sharply bent DNA is more flexible than expected, possibly due to the excitation of flexible defects. However, the existence and properties of these defects have been debated for two decades because of the difficulty in observing and measuring such defects. Here, we performed Brownian dynamics simulations using a DNA model, oxDNA, and observed equilibrium defect excitation in small DNA circles. By analyzing thousands of spontaneous defect excitation and annihilation events, we extract the excitation energy Ed and defect flexibility. We find that Ed ranges from 13 to 18 k_BT , depending on the ionic strength, AT/CG content in sequence, and temperature. Using these defect parameters, we quantitatively explained four sets of experimental results: (i) abnormally high occurrences of DNA large bending in AFM experiments; (ii) abnormally high looping probability of short DNA fragments; (iii) sequence dependence of DNA loop probability; (iv) relatively weak electric field for nanopore translocation of a DNA knot.

Keywords: DNA mechanics, Molecular dynamics

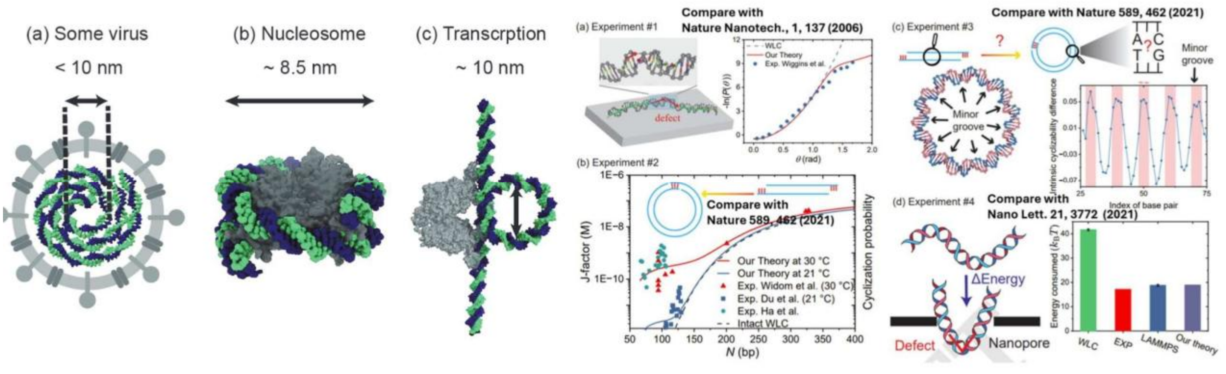

Figure 1. *(left)DNA sharp bending in living organisms. (right) Comparison with four types of experiments with our theory.*

References

[1] Quantifying Flexible Defect Excitation in Sharply Bent DNA 2025 Under peer

Continuity of Short-Time Dynamics Crossing the Liquid–Liquid Phase Separation in Charge-Tuned Protein Solutions

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Liquid–liquid phase separation (LLPS) constitutes a crucial phenomenon in biological self-organization, not only intervening in the formation of membraneless organelles but also triggering pathological protein aggregation, which is a hallmark in neurodegenerative diseases. Employing high-resolution incoherent quasi-elastic neutron spectroscopy (QENS), we examine the short-time self-diffusion of a model protein undergoing LLPS as a function of phase splitting and temperature to access information on the nanosecond hydrodynamic response to the cluster formation both within and outside the LLPS regime [1]. We investigate the samples as they dissociate into microdroplets of a dense protein phase dispersed in a dilute phase as well as the separated dense and dilute phases obtained from centrifugation. By interpreting the QENS results in terms of the local concentrations in the two phases determined by UV–vis spectroscopy, we hypothesize that the short-time transient protein cluster size distribution is conserved at the transition point while the local volume fractions separate (Figure 1). The presentation will provide insights into the colloid picture of protein solutions (Refs. [1,2] and references therein) and illustrate recent progress in neutron spectroscopy and associated data analysis.

Keywords: short-time self-diffusion, liquid-liquid phase separation, crowding

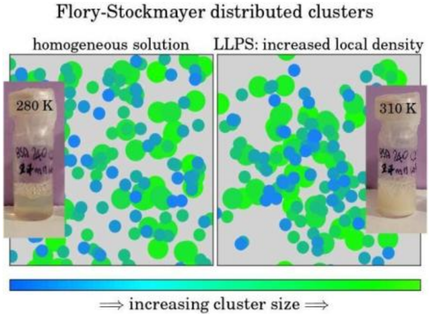

Figure 1. *The schematic illustrates the cluster distributions outside (left) and within the LLPS regime (right) with local dense and dilute regions described by the Flory–Stockmayer model [1]. The inset photographs display the associated protein solution in the visually transparent (left) and turbid (right) states, the transition being achieved by warming from 280K to 310K.*

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Self-organization and memory in randomly driven disordered materials

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We consider self-organization and memory formation in a mesoscopic model of an amorphous solid subject to a protocol of random shear confined to a strain range ±ε_{max}. We develop proper read-out protocols to show that the response of the driven system self-organizes to retain a memory of the strain range, which can be subsequently retrieved. Our findings generalize previous results obtained upon oscillatory driving and suggest that self-organization and memory formation of disordered materials can emerge under more general conditions, such as a disordered system interacting with its fluctuating environment. Self-organization results in a correlation between the dynamics of the system and its environment, providing thereby an elementary mechanism for sensing. We conclude by discussing our results and their potential relevance for the adaptation of simple organisms lacking a brain to changing environments.

Keywords: memory, self-organization, elasto-plastic model,

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Understanding and mimicking cryopreservation of living cells: in situ observation of freezing of lipid vesicles

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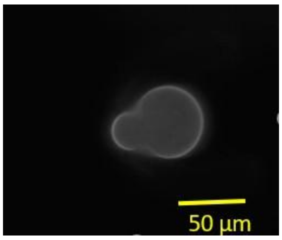
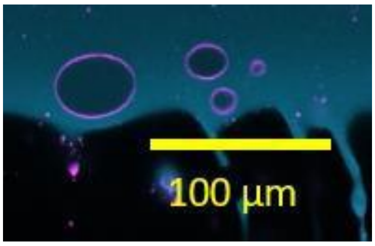
Cryopreservation of cells is a major issue in medicinal application. The rate of survival depends on the freezing velocity [1] but the mechanisms at play leading to cell damage are not fully understood yet. During the growth of ice crystals, the segregation of solutes close to the ice crystals creates strong gradients of solutes which can lead to dramatic changes of the cell volume by permeation of the solvent through their permeable membrane. Hence, the permeability of membranes is a very important factor to try to understand the key factors involved in the survival rate of cells.

In our work we study the freezing of lipid vesicles and study the influence of their permeability on the freezing process. We use microfluidic chips to trap the liposome and measure their permeability to water and other solutes during osmotic shocks combining Fluorescence exclusion microscopy as well as standard fluorescence microscopy [2]. (image 1a).

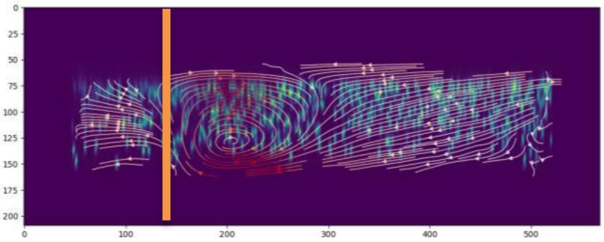
Furthermore, we use confocal microscopy to study in situ interaction between a growing ice front and liposomes in a controlled temperature gradient [3]. We observe the deformation of the objects as the approach the ice front (figure 1 b). We show that these effects are linked to the solute concentration gradient near the front as the solute (sucrose) is rejected by the ice front. Moreover we evidence recirculation flows due to density differences caused by the accumulation of sucrose close to the ice front. Using PIV (particle image velocimetry) we show that the amplitude of the convection rolls depends on the sucrose concentration and velocity of the ice front(figure 1c).



1a) Shrinked vesicle in a microfluidic trap



1b) deformed vesicle approaching the ice front



1c) PIV analysis of the flow near the ice front (particles in green, ice front delimited by the orange line)

Keywords: freezing, liposomes, solute gradients

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How Macromolecular Crowding Shapes Bivalent Binding and Cooperativity

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Macromolecular crowding plays a crucial role in various biophysical processes, including diffusion [1], gene expression [2,3], and cell growth [4]. However, its effects on multivalent binding—and particularly on cooperativity—remain poorly understood. In this talk, we will examine how crowding influences the binding of monovalent ligands to divalent biomolecules [5]. Using scaled particle theory in combination with a computational framework that integrates Brownian dynamics and Monte Carlo simulations, we reveal that crowding can dramatically modulate cooperativity, either enhancing or suppressing it, depending on molecular size and conformational changes. Specifically, we show that cooperativity increases when a divalent molecule expands upon binding the first ligand and contracts upon binding the second. We also demonstrate that crowding can facilitate binding events that would not occur in dilute solutions. As a case study, we employ a coarse-grained immunoglobulin G (IgG) model [6] to investigate IgG-antigen interactions, showing that crowding enhances IgG cooperativity in bulk solutions but reduces it when IgG binds antigens on a surface [5]. These findings provide new insights into the fundamental role of macromolecular crowding in biological systems and may have implications for immunology and drug design.

Keywords: macromolecular crowding; diffusion; binding cooperativity; multivalent biomolecules; immunoglobulins.

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How does mucus rheology affect mucociliary clearance?

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The airways are protected by mucus, a complex fluid transported along the epithelial surface, from the lungs to the throat, by the coordinated beating of millions of microscopic cilia. This process is known as mucociliary clearance. Dysfunction of this mechanism is associated with all chronic respiratory diseases and in particular obstructive ones, where mucus accumulation leads to the airway obstruction.

The aim of this study is to understand how mucus rheology affects mucociliary clearance and its role in obstructive phenomena. In vitro experiments are carried out on air-liquid interface (ALI) cultures of bronchial epithelium. While mucus swirls are observed, transport efficiency and microrheology measurements are performed using traceable fluorescent beads. The transport properties of healthy native mucus are compared to those of an artificial mucus of controlled rheology.

We show that native mucus displays elastic behaviour up to a critical flow rate, which is reached through hydration. At this point, viscoelastic behaviour emerges. The comparison between native and artificial mucus shows that native mucus stops flowing for lower elastic modulus than the artificial one. We conclude that rheology itself cannot explain obstructive phenomena and discuss other parameters that should be considered. Our findings provide new insights into the biophysical parameters that govern mucociliary clearance.

Keywords: Mucus, microrheology, in-vitro experiments

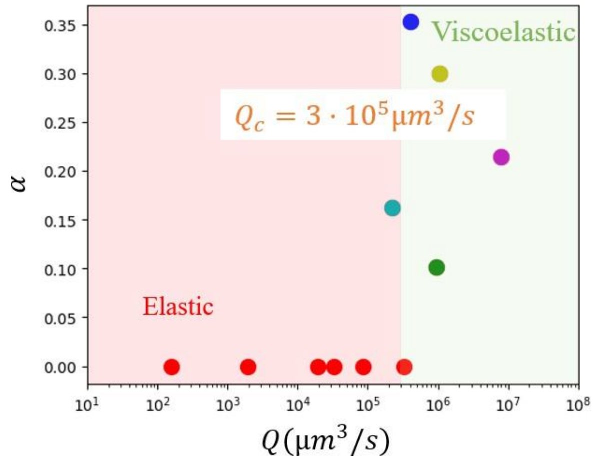

Figure 1. *Slopes of microrheological curves (α) according to the mucus flow rate (Q), revealing a transition from an elastic to a viscoelastic regime.*

Tuesday 30th September 2025

M. Experimental & Computational Methods (including AI)

(Room 3)

The Countoscope: Quantifying Dynamics by Counting Particles in Boxes

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Quantifying the dynamics of particle suspensions is a widespread interest in soft matter. For instance, probing the motion of cells or larger organisms can help us understand biological behavior. When multiple particles interact, they perform collective dynamics, which visually translates into a zoology of effects, including dynamic aggregation to ensemble and directed motion. Yet, available analysis techniques face challenges reconstructing trajectories in dense suspensions where accurately labelling particles is difficult. In addition, most realistic systems include boundaries, such as of membranes or pores, which modifies local transport properties. Tracking methods also struggle with such system heterogeneities.

Inspired by Smoluchowski, we introduce a broadly applicable analysis technique, that probes particle dynamics based on a simple principle: counting the fluctuating number of particles in finite observation boxes of an image. Through colloidal experiments, simulations, and theory, we demonstrate the practical benefits of analyzing fluctuating counts. We can determine equilibrium motion properties, such as self-diffusion coefficients [1]. Moreover, by increasing the observation box size, we can naturally probe collective diffusion coefficients [2]. Out-of-equilibrium features also manifest in such fluctuating counts: for instance, our framework is sensitive to self-propulsion velocities. Beyond, by correlating nearby boxes we demonstrate how to map out flow field maps.

Both in dense or heterogeneous states, by simply counting particles, we overcome challenges of trajectory reconstruction. We explore our framework on various suspensions where particle coordinates can be resolved, from ions to active and biological particles such as bacteria. The "Countoscope" offers the unique possibility of systematically linking individual and collective behavior, opening up broad perspectives in soft and statistical physics.

Keywords: colloids, diffusion, microscopy, flow fields, suspensions

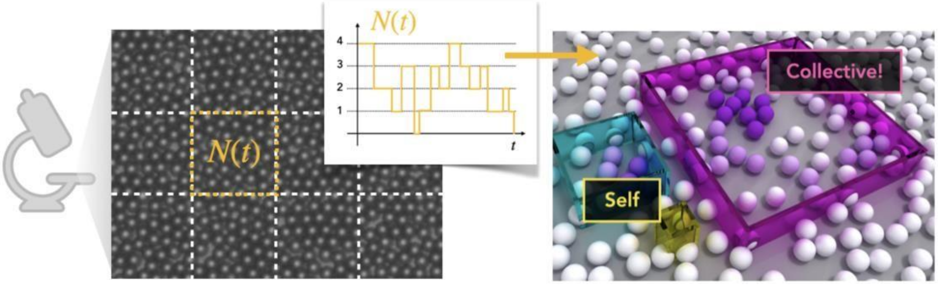

Figure 1. *Virtual observation boxes on a bright-field image of a dense 2D colloidal. The number of particles in a box fluctuates with time. We extract relevant kinetic properties from these fluctuating counts.*

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Analysing the Effect of Noise on Static and Dynamic Results from Total Internal Reflection Microscopy (TIRM)

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Total internal reflection microscopy (TIRM) has been used for about 30 years to measure interaction potentials between suspended spherical colloids and flat surfaces [1]. The method also allows measuring position resolved dynamic properties, specifically the diffusion coefficient and the drift velocity normal to the surface. However, in literature there are reports on dynamic results which are at conflict with expectations from standard hydrodynamics. In this work, we have used experimental TIRM in conjunction with molecular dynamics simulations to investigate the effects of inherent error sources due to noise artifacts [2,3] on TIRM results. We find that detector shot noise and too long sampling times may cause erroneous results in the steep parts of the interaction potential. Further, the noise does not significantly affect dynamic data, but we find that too long sampling times and/or too small probe particles will cause issues. Additionally, we observe that dynamic results are very likely to differ from the standard hydrodynamic predictions for stick boundary conditions. Thus, to minimize experimental errors, sampling times and particle sizes have to be properly chosen when designing TIRM experiments and for the analysis of dynamic information, partial slip conditions have to be considered.

Keywords: Total internal reflection microscopy (TIRM); colloidal interaction; Brownian dynamics, hydrodynamic interaction

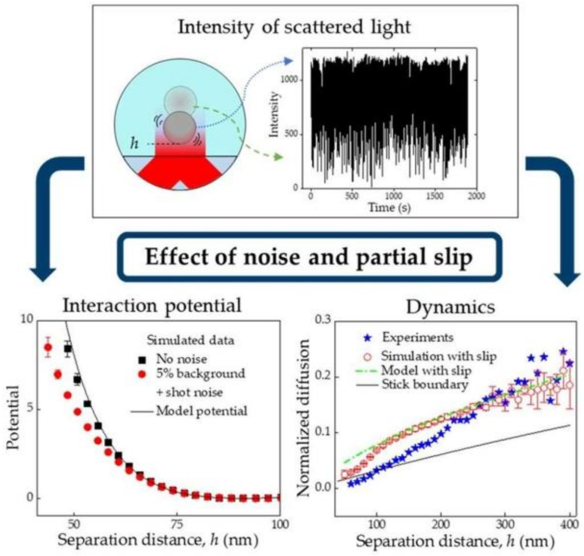

Figure 1. *The effect of noise on static and dynamic TIRM*

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Dynamical and structural signature of the glass transition in soft colloids

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Despite several decades of research, the physics of glass formation remains an outstanding unsolved question in condensed matter physics [1]. Glass transition is characterized by a spectacular slowing down of the dynamics, but at the same time the glass undergoes only minute structural changes, preserving the same structure of a disordered liquid [2]. In this context structure-dynamics correlation is one of the major ongoing debates in the glass transition.

In this talk we will investigate this point reporting very recent simultaneous in situ Small-Angle Neutron Scattering (SANS) and Dynamic Light Scattering (DLS) measurements on a thermo responsive microgel of poly(N-isopropylacrylamide) (PNIPAM) and a multi-responsive microgel composed of Interpenetrating Polymer Networks (IPN) of PNIPAM and poly(acrylic) acid. The measurements have been obtained through the use of a new SANS-DLS setup implemented by our group and shown in Figure 1 [3]. When installed on a SANS beamline the setup permits complementary and simultaneous information on the microscopic structure (through SANS) and dynamics (through DLS) of soft matter systems to be acquired. In this way the slowing down of dynamics and the corresponding changes in the structure of PNIPAM and IPN samples have been obtained varying sample concentration and temperature. At variance with expectations of a paradoxical discrepancy between structure and dynamics during the process of glass formation, the two parameters well correlate. The possibility to follow exactly at the same time and on the same sample the dynamics and structure of a colloidal sample opens up new possibilities in the comprehension of complex systems and out of equilibrium states.

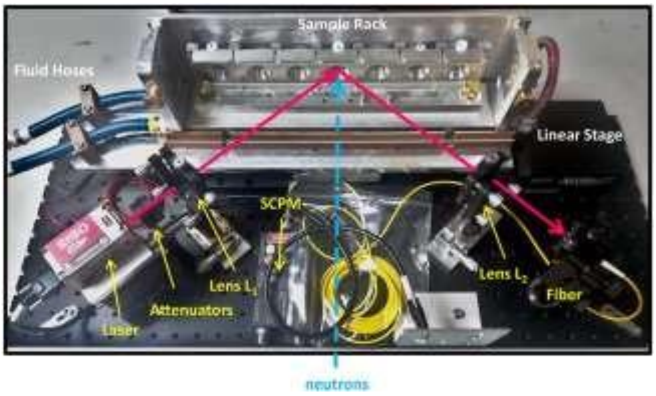

Figure 1. *Photograph of the DLS-SANS apparatus. The red arrows indicate the path of the laser beam, while the dashed cyan arrow indicates the path of the neutron beam. From Ref. [3].*

Keywords: Microgel, dynamical behaviour, structural behaviour, glass transition.

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Hydrodynamic fluctuations in sedimenting colloids

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Under gravity, colloidal suspensions establish a steady-state concentration profile where diffusion balances sedimentation. This equilibrium, famously studied by Perrin in experiments that supported Einstein's theory of Brownian motion [1], provided compelling evidence for the molecular nature of matter and earned Perrin the 1926 Nobel Prize in Physics [2]. While Einstein's theory applies to dilute systems with negligible interactions, sedimented samples often reach concentrations where particle interactions and hydrodynamic coupling become significant. In this regime, it is crucial to distinguish between *self-diffusion*, the random motion of individual particles, and *collective diffusion*, which governs the relaxation of concentration fluctuations driven by density gradients. Modern particle-tracking approaches can access self-diffusion at sedimentation equilibrium. However, probing collective dynamics would require space-resolved Dynamic Light Scattering to resolve the relaxation of concentration Fourier modes in a vertically stratified sample, a technically demanding approach that has not yet been realized.

To overcome this limitation, we employed Differential Dynamic Microscopy [3], which analyzes temporal fluctuations in Fourier components of microscopy images and enables depth-resolved measurements across a wide wave-vector range q. At large q, the dynamics match those observed in homogeneous suspensions at the same local concentration, consistent with classical diffusion and hydrodynamic interactions [4]. At small q, however, relaxation occurs faster than expected due to buoyancy-driven amplification of long-wavelength concentration modes. This behavior strikingly resembles that observed in non-equilibrium processes such as thermophoresis [5], despite the system being at thermodynamic equilibrium. Moreover, in sufficiently thin samples, we observe the re-emergence of diffusive-like relaxation at even smaller q, governed by a distinct diffusion coefficient. These findings reveal previously unexplored aspects of collective dynamics in sedimented colloidal suspensions, remarkably overlooked for over a century despite the ubiquity of sedimentation in natural, industrial, and laboratory settings.

Keywords: colloidal suspensions, sedimentation, hydrodynamic interactions, microscopy.

Acknowledgements: This work was partially supported by the Austrian Science Fund (FWF), grant number M 3250-N.

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Measuring electric charging and discharging of individual aerosol particles with optical tweezers

A. Stoellner[1], *I.C.D. Lenton*[2], *C. Muller*[1] *and S.R. Waitukaitis*[1]

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Charge accumulation on aerosol particles, e.g. dust, volcanic ash or cloud ice, plays a critical role in a variety of natural and industrial processes [1]. In our experiment, we utilize optical tweezers to levitate individual aerosol particles in the micrometer size range and observe their charging and discharging dynamics over days-to-weeks time periods and with elementary-charge resolution. Our approach allows us to study these processes without losing information to ensemble averages or external interference from other particles or substrates [2], and is applicable to solid and liquid particles in the micrometer size range. Using multi-photon absorption from the trapping laser [3] we can charge the trapped particle at different rates and to different values, observing every charging and discharging event along the way. Additionally, the experiment allows us to control the relative humidity around the particle and to fully discharge the particle using air ions. By studying the charging behavior of the particle and the spontaneous discharges it experiences, we hope to contribute to a better understanding of the microphysical processes involved in lightning initiation and adjacent electrical phenomena in the atmosphere.

Acknowledgement

This project has received funding from the European Research Council (ERC) under the European Union's Starting Grant (A. Stoellner, I.C.D. Lenton & S.R. Waitukaitis received funding from ERC No. 949120, C. Muller received funding from ERC No. 805041).

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Photon correlation methods using MHz hard X-ray FEL radiation

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The European X-ray Free Electron Laser (EuXFEL) generates ultra-short and coherent hard X-ray pulses with Megahertz repetition rate, providing unique opportunities for coherent scattering and imaging experiments. This talk introduces the Materials Imaging and Dynamics (MID) instrument at EuXFEL [1] by highlighting two experimental campaigns utilizing these special beam properties and the available instrumentation.

Crystallization, one of the most fundamental phase transitions, is in many respects challenging to study in atomic and molecular liquids because of the spontaneous nature of the process and the very short timescales and small lengthscales involved. Combining micrometer-wide liquid jets, which rapidly super-cool and crystallize when injected into vacuum, together with femtosecond Xray scattering, allows probing this process at the very first nucleation events and overcoming ensemble averages involved in conventional X-ray scattering experiments. This serial diffraction approach presents the to-date most stringent test of classical nucleation theory in noble-gas liquids of Krypton and Argon [2]. Additionally, it opens up the possibility to follow deviations from ideal crystal structures, such as stacking faults and twinning, by employing X-ray Cross Correlation Analysis (XCCA) [3].

Due to the MHz repetition rate of EuXFEL, dynamics can be measured on nanometer length- and sub-µs time-scales by employing X-ray Photon Correlation Spectroscopy (XPCS) [1,4] in smallangle scattering geometry (SAXS). This covers the spatio-temporal range of diffusion processes in dense cellular environments, but also the first stages of aggregation and phase transition phenomena in many soft matter systems. We will introduce the hard- and software implementations to establish an experimental pipeline, which is available for users of the beamline as standard configuration (SAXS-XPCS). Experiments using this setup cover e.g. aggregation of antibody proteins [5], temperature-jump phase transitions of stimuli-responsive polymers [6], or studying the effect of molecular crowding on dense protein solutions [7].

Keywords: X-ray scattering, XFEL, XPCS, SAXS, XCCA

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Neural functionals in statistical mechanics

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Classical density functional theory is a formally exact framework for the description of fluids and soft matter in thermal equilibrium. We demonstrate that simulation-based machine learning of neural networks is an effective computational method to overcome the difficulty of finding the functional mappings that are required in applications. Predictions of neural density functionals supersede state-of-the-art analytic treatments in accuracy and remain feasible for multiscale problems that far exceed the training data [1]. Neural functional calculus gives efficient access to structural and thermodynamic properties, which is particularly relevant for investigating liquid-gas phase coexistence and associated phenomena [2]. Besides being extensible to nonequilibrium systems [3], neural functionals can also be generalized to predict complex observables, such as cluster statistics [4], and to solve topical inverse design problems in soft matter physics [5].

Keywords: neural functionals, machine learning, classical density functional theory, phase separation, inverse design, nonequilibrium

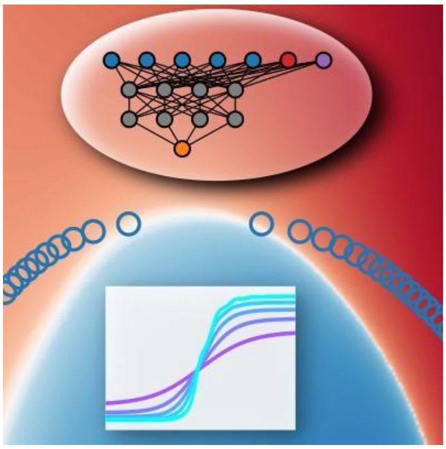

Figure 1. *Neural functionals allow one to address a wide range of phenomena in fluids and soft matter, including their structure [1,2], phase behaviour and interfacial properties [2], as well as to investigate nonequilibrium flow [3], general observables [4] and inverse design tasks [5].*

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Accelerating particle-scale numerical simulations via convolutional neural networks

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Machine learning (ML) is increasingly transforming scientific research, yet its application to suspension rheology remains limited [1]. Recent efforts have leveraged data-driven and physicsinformed ML techniques to improve constitutive modeling and accelerate simulations [2-5], but a unified ML framework is still lacking. Further integration of ML could significantly enhance predictive accuracy and computational efficiency [6].

In this work, we accelerate particle-scale simulations by integrating convolutional neural networks (CNNs) into the Fictitious Domain Method (FDM) [7]. The FDM models the flow of a Newtonian fluid over a meshed domain containing rigid, neutrally buoyant spheres. In the Stokes regime, where inertia is negligible, fluid velocity and pressure satisfy the modified Stokes equations, in which a force density field plays the coupling role between fluid and particles. Rigid body motion is enforced within each particle's volume, and both long- and short-range hydrodynamic interactions are computed taking care of lubrication.

A key computational challenge is obtaining the correct force density field, which traditionally requires iterative updates until convergence. We replace this step with a CNN that directly predicts it from the flow field and particle states. This eliminates costly iterations, significantly accelerating simulations while maintaining accuracy.

To validate our approach, we first apply the CNN to benchmark cases, demonstrating its ability to reproduce force distributions and particle motions with high fidelity. We then showcase its effectiveness in large-scale particle simulations, highlighting substantial computational speedups while preserving reliability.

By integrating ML into the FDM framework, this work provides a novel and efficient approach to simulating suspensions. Our method enhances computational efficiency and opens new avenues for studying complex suspension flows, advancing both numerical modeling and our understanding of rheological behavior.

Keywords: numerical simulations, convolutional neural networks, machine learning

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Physically motivated mesoscale approaches for the predictive mechanical design of dynamic elastomers and gels

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The consummate goal of predictive material design is to accurately extrapolate a material's properties at application scales, based solely on its molecular composition and *ab initio* synthesis. In the field of polymer mechanics, we aim to optimize bulk mechanical properties of elastomers and gels for applications such as tissue engineering, additive manufacturing, and soft actuation. Optimization of polymers without undue experimental cost requires the inventive use of computational models, due to their extensive parametric design spaces. These must relate polymers' emergent mechanics (at spatiotemporal scales up to millimeters and weeks) to their constituents' dynamic arrangement (at scales down to angstroms and femtoseconds). This inherently multiscale problem is addressed by first principles-anchored quantum mechanical or molecular dynamics (MD) models at atomic to molecular scales, and thermodynamically consistent constitutive models at continuum scales. However, between these regimes reside spatiotemporal domains too large for conventional MD interrogation, but at which stochastic localization processes and steep gradients hinder the use of homogenized continuum models. To bridge this gap, we introduce a novel class of coarse-graining methods that model dynamically crosslinked elastomers and gels based on physically-motivated statistical mechanics relations. These models significantly reduce computational costs over conventional coarse-grained MD, while preserving detail about network topology and predicting mechanical responses in agreement with continuum theory and experiments. Thus, we believe that these methods and their offshoots may constitute a significant tool in the arsenal for predictive polymer design.

Keywords: Dynamic polymers, network mechanics, computational mechanics, viscoelasticity., mesoscale models

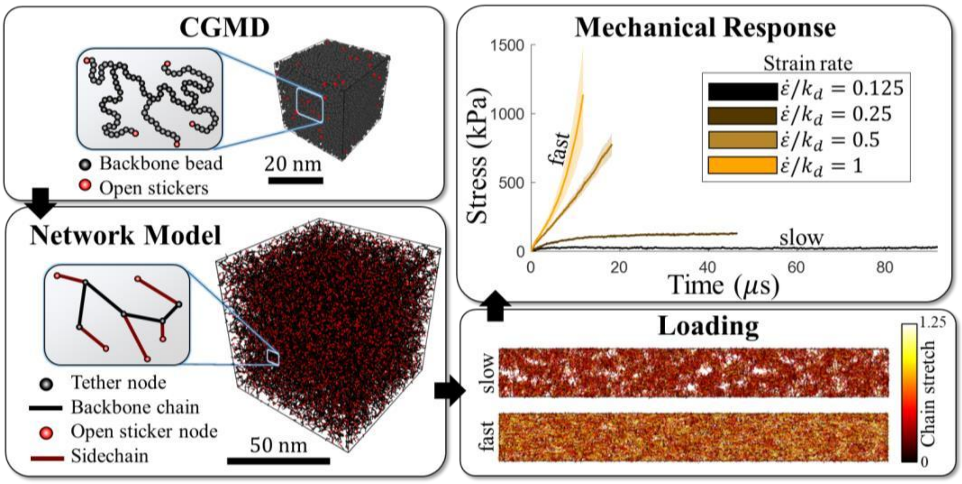

Figure 1. *Mesoscale network models for accessing microscale mechanical responses of dynamic polymers.*

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Inferring effective interactions from the structures of active Brownian particles

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Keywords: active Brownian particles, effective interactions, inverse method, test particle insertion

We present an approach to obtain effective pair potentials which describe the structure of two-dimensional systems of active Brownian particles (ABPs). The particle arrangements are obtained from active molecular dynamics simulation. The effective pair potential is found by an inverse method, which matches the radial distribution function found from two different methods. The inverse method has been previously demonstrated using simulated equilibrium configurations of passive particles [1]. We have now applied the method to active particle structures.

Interestingly, although active particles are inherently not in equilibrium, we can still obtain effective interaction potentials which accurately describe the structure of the active system. Furthermore, treating these potentials as equilibrium ones allows us to measure the effective chemical potentials and pressures. Both the passive interactions and active motion of the active Brownian particles contribute to their effective interaction potentials.

Purely repulsive passive interactions give particularly insightful effective pair potentials, since these contain attractive wells (see Figure 1): this is a clear demonstration of the emergent attractive behaviour of ABPs. Furthermore, the shape, such as the depth, of these attractive wells offers a means to quantify this emergent behaviour.

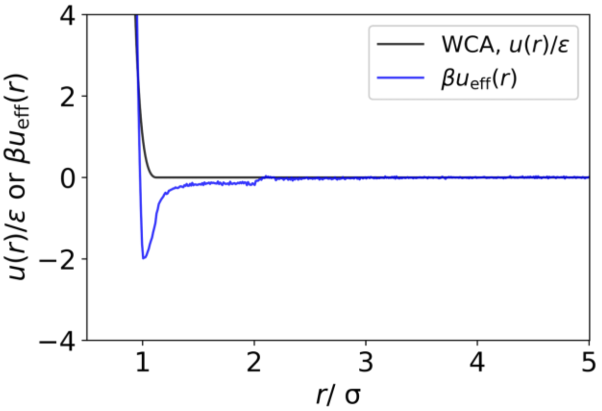

Figure 1. *Effective interaction potential for active particles (blue line) compared with the underlying passive Weeks– Chandler–Anderson (WCA) potential (black line). Distances are scaled by the particle diameter, σ, and energies by ε or the thermal energy ($\beta = 1/kT$).*

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Python-JAX-based Fast Stokesian Dynamics with Neural Networks

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Stokesian Dynamics is a powerful computational framework for simulating the motion of particles in a viscous Newtonian fluid under Stokes-flow conditions. Traditional implementations can be computationally expensive to use, as they rely on the inversion of large mobility matrices to determine hydrodynamic interactions. Recently, however, the simulation of thermalized systems with large numbers of particles has become feasible [1]. Their "fast Stokesian dynamics" method leverages a saddle-point formulation to ensure overall scaling of the algorithm that is linear in the number of particles; performance relies on dedicated GPU computing.

Here, we present a different route toward implementing fast Stokesian dynamics, which instead leverages the Just-in-Time compilation capabilities of Google JAX. We refer to this implementation as JFSD [2] and show that it both has the right scaling and is sufficiently fast by the standards of modern computational physics. Looking toward the future of simulating hydrodynamic effects in particle suspensions, we propose a hybrid framework that replaces Stokesian dynamics' full many-body computations with a neural network trained on JSFD generated data. That is, we base our algorithm on the pairwise Rotne-Prager-Yamakawa method, introducing the many-body effects via the neural network, thereby avoiding costly matrix inversions. We demonstrate the potential of this method on a simple system, which reveals that we capture the desired many-body effects at a fraction of the cost of using JFSD. We conclude that by combining foundational methods with innovative computational techniques, the future of Stokesian dynamics is looking bright.

Keywords: Computational Fluid Dynamics, Machine Learning, Rheology

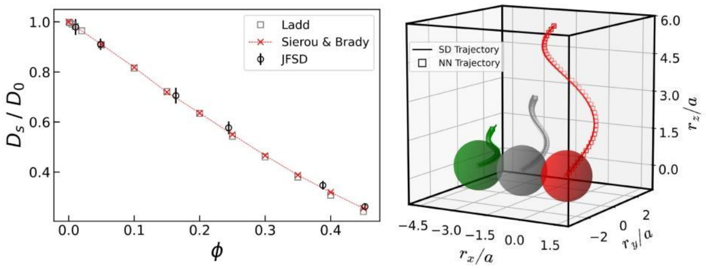

Figure 1. *(left) The reduced short-time self-diffusion coefficient of a hard-sphere suspensions as a function of volume fraction. (right) Example trajectories obtained using our neural-network-enhanced Rotne-Prager-Yamakawa solver.*

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Phase-field simulations elucidate bijel formation mechanism during solvent transfer-induced phase separation

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Solvent transfer-induced phase separation (STrIPS) enables scalable synthesis of bicontinuous interfacially jammed emulsion gels (bijels), a soft material with applications in membrane separation, catalysis and energy storage [1]. However, limited options for *in-situ* observation of bijel formation during STrIPS currently hinder our understanding on how phase separation dynamics influence the resulting bijel structure. While computer simulations can help bridge this gap, the relevant spatial and temporal scales of the STrIPS process (hundreds of micrometers over seconds) are not readily accessible to conventional bijel simulation methods (e.g. Lattice-Boltzmann). In this research, we overcome this issue by introducing a phase-field (PF) model for STrIPS-bijel formation [2]. We demonstrate that the complex STrIPS process can be simulated by separately considering its core components: solvent diffusion, phase separation and nanoparticle adsorption. In particular, we show that the interfacial tension (IFT) serves as an effective substitute measure for the presence of nanoparticles in PF-STrIPS simulations.

Next, we validate the results of the PF-model through comparison with experimental STrIPSbijel structures, acquired *via* confocal laser scanning microscopy. Not only do the simulated and experimental bijel morphologies show strong qualitative agreement, the PF-model is additionally able to relate observed morphological trends in the experimental system to differences in the relative dynamics of phase separation with respect to solvent diffusion.

In conclusion, this research presents a novel PF-method for the simulation of bijel formation via STrIPS. By providing unique insights into the formation mechanisms of current STrIPS-bijel morphologies, it paves the way for designing the next generation of functional bicontinuous materials.

Keywords: Phase-field simulation, bicontinuous emulsion, nanoparticles

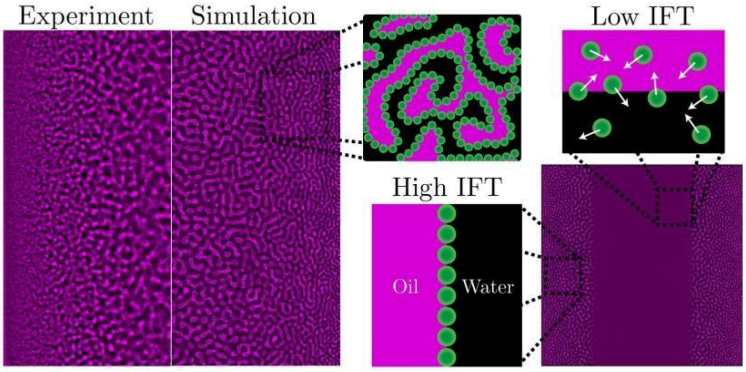

Figure 1. *Using the IFT as a substitute measure of nanoparticle adsorption, STrIPS-bijel formation can be accurately captured by a PF-model, showing strong agreement between simulated and experimental morphologies.*

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Generative BigSMILES: an extension for polymer informatics, computer simulations and ML/AI

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Representing the intrinsic stochasticity of polymeric materials remains a challenge for traditional line notations such as InChi or SMILES, which are typically designed for single, well-defined molecules. BigSMILES[1] is a widely adopted alternative to represent polymer structures in a line notation readable by both machines and humans. BigSMILES extends the functionality of SMILES by portraying a polymer as a sequence of interconnected monomers. However, it lacks information about the likelihood of each possible polymer structure that can arise from a BigSMILES string.

Building on the BigSMILES framework, we introduce Generative BigSMILES[2] (GBigSMILES)—a compact extension that encodes ensemble-level information such as molecular weight distributions, reactivity ratios, and ensemble sizes. This enhancement enables the specification of polymer ensembles with assigned structure likelihoods, addressing the limitations of purely descriptive representations. G-BigSMILES retains compatibility with the original BigSMILES notation and supports both the generative construction of simulation-ready molecular ensembles and the probabilistic evaluation of candidate molecules, thus bridging the gap between polymer representation and informatics-driven design. Moreover, our G-BigSMILES implementation (https://github.com/InnocentBug/G-BigSMILES) includes the generation of a corresponding reaction graph representation, suitable for machine learning models based on graph neural networks.

In this presentation, the G-BigSMILES notation will be described with special emphasis on its generative nature and its utility as a detailed descriptor of polymer materials. Then, its potential as a tool for automated workflows in simulation and experimentation, as well as for machine learning representations, will be discussed.

Keywords: Polymer informatics, graph neural networks, stochastic generation

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In Silico Prediction of Multi-Component Functional Material Formulations via Machine Learning Coupled with Molecular Simulation

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This study focuses on the prediction and optimization of cleansing foam formulations, which are representative multi-component functional materials with a high degree of compositional complexity. The vast combination of potential ingredients presents significant challenges in developing effective predictive models [1]. To address this, we constructed a machine learning (ML) framework to estimate cleansing performance based on ingredient ratios. Additionally, we integrated molecular-level descriptors extracted from dissipative particle dynamics (DPD) simulations to enhance prediction accuracy by reflecting self-assembly behaviors of surfactants and structural properties [2].

The proposed model was validated using three evaluation strategies: points out, mixtures out, and compounds out. The "points out" method, which involves random data splitting, showed the highest performance ($R^2 = 0.718$) when using both modeling and simulation-derived features. In the "mixtures out" method, where the model is tested on unseen ingredient combinations with known raw materials, the performance improved from $R^2 = 0.531$ to 0.655 with simulation features. In contrast, for the "compounds out" scenario, involving entirely novel raw materials, all R^2 values remained negative, indicating a current limitation in generalizing beyond known surfactant types.

These findings demonstrate that integrating molecular simulations into ML pipelines can improve predictive accuracy for complex formulations, particularly in cases involving nonlinear ingredient interactions. However, generalization to unknown materials remains a key challenge. To address this, future efforts will focus on expanding the chemical diversity of the dataset and incorporating additional descriptors such as molecular polarity, hydrogen bonding potential, and pH sensitivity, which are expected to significantly influence surfactant behavior and formulation efficacy.

This combined approach offers a promising pathway toward data-driven formulation development in the cosmetic and materials industries, enabling faster and more sustainable product innovation. It also contributes to reducing experimental costs and minimizing the environmental impact associated with trial-and-error formulation processes.

Keywords: Machine Learning, Molecular Simulation, DPD, QSPR

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Interpretable machine-learning enhanced parametrization methodology for Pluronics-Water Mixtures in DPD simulations

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Pluronics, or poloxamers, represent a peculiar class of soft matter systems characterized by their amphiphilic triblock structure, consisting of a hydrophobic poly(propylene oxide) (PPO) core flanked by two hydrophilic poly(ethylene oxide) (PEO) chains. Their versatility, biocompatibility, temperature sensitivity, and self-assembly capabilities make them suitable for applications such as drug delivery [1]. Depending on factors like hydrophilic-lipophilic balance (HLB), concentration, temperature, and shear stress, Pluronics can exist as unimers or self-assemble into micelles and supramolecular aggregates, encapsulating hydrophobic drugs within the PPO core.

Key properties such as Critical Micellar Concentration (CMC), micelle radius (R_g), and aggregation number (A_s) significantly impact functionalities like drug delivery. Although accurately predicting these properties is crucial, experimental approaches are often costly and time-consuming.

Coarse-grained methods, such as Dissipative Particle Dynamics (DPD), are powerful tools that complement experiments and facilitate the rational design and performance optimization of materials for specific applications. By bridging the gap between atomistic and macroscopic scales [2], they effectively capture material morphologies and their impact on macroscopic behavior. However, selecting appropriate DPD model parameters to ensure accurate predictions remains challenging.

We address this challenge by combining Gaussian Process Regression (GPR) as a surrogate model for DPD simulations with SHAP (SHapley Additive exPlanations) analyses to enhance parameterization of Pluronic systems. This top-down strategy, integrating data-driven methods and interpretability techniques, not only facilitates parameterization but also provides valuable insights into the impact of input parameters.

The GPR model serves as an effective surrogate for DPD simulations, efficiently handling small datasets while providing uncertainty estimates. SHAP analysis further improves interpretability, revealing how each parameter influences output properties. An adaptive grid-search strategy iterates to optimize DPD parameters, accurately capturing relevant properties for four Pluronic types: L64, P65, P104, and F68. These results lay the foundation for transfer learning to extend parameterization across diverse Pluronic systems and conditions.

Keywords: Soft Matter, Amphiphilic Copolymers, Coarse-grained modeling, Parameter Optimization, Machine learning, Surrogate Modeling.

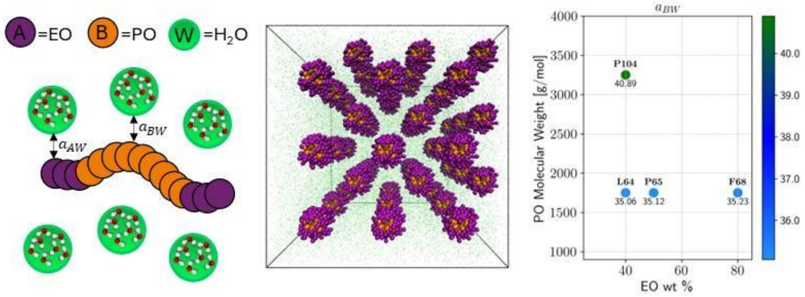

Figure 1. *Optimization of DPD model parameters for Pluronic systems.*

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Study of Polymer Nanocomposites Through Simulations and ML Methods: From Atoms to Macroscopic Properties

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The computational study of complex polymeric materials is a very challenging field, due to the broad spectrum of the underlying length and time scales. We present a hierarchical multi-scale methodology for predicting the macroscopic properties of polymer-based nanostructured systems, which involves atomistic simulations, coarse-grained models, homogenization approaches and continuum models [1-3]. The CG and the continuum models are derived through a systematic "bottom-up" data-driven strategy, using information from the atomistic scale without any adjustable parameter [1]. Moreover, Deep Learning algorithms are developed to reintroduce atomic detail on the CG scale and obtain atomistic configurations of long polymer chains [1].

The proposed computational methodology is applied to provide a fundamental understanding of the mechanism of mechanical reinforcement in glassy polymer nanocomposites, which is of paramount importance for their tailored design. We present a detailed investigation of the coupling between the density, structure and conformations of polymer chains with respect to their role in mechanical reinforcement [2-3]. We found that the effective mass density and rigidity of the matrix region change with filler volume fraction, while that of the interphase remains constant. The origin of mechanical reinforcement is attributed to the heterogeneous chain conformations in the vicinity of the nanoparticles, which involve a twofold mechanism. In the low-loading regime, the reinforcement comes mainly from a thin, single-molecule, 2D-like layer of adsorbed polymer segments on the nanoparticle, whereas in the high-loading regime, the reinforcement is dominated by the coupling between train and bridge conformations; the latter involves segments connecting neighboring nanoparticles.

Keywords: Multi-scale simulations, Polymer nanocomposite, Machine Learning algorithms

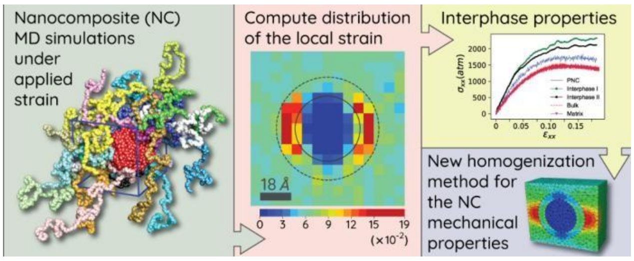

Figure 1. *From atomic scale to macroscopic properties of polymer nanocomposites: A nano-micro-macro approach involving for predicting the heterogeneous mechanical behavior of complex systems [3]*

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Combined Methods Rheo-Spectroscopy: Rheo-IR Development and Examples

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Macroscopic mechanical properties are often determined, or influenced by the underlying molecular structures. Such molecular structures can be crystallites, agglomerates, topology of polymer chains, functional chemical groups, dipole moments in the molecules, or newly breaking and forming chemical bonds. Understanding the molecular structures, and possible changes in them, and subsequently understanding the effect this has on the macroscopic properties of the material, such as rheology, is of interest in many different fields of research, such as e.g., polymers, colloids, food science and cosmetics.

Such correlated information would open up new possibilities in the field of creating materials, where a designed molecular structure would lead to desired macroscopic property. Such structure property relationships, can be analyzed with combined methods, that allow simultaneous acquisition of mechanical rheological and molecular spectroscopical information, which then allows correlating the acquired information of different length scales.

Combined methods are developed and frequently used in the polymeric materials group. Now these combinations are available e.g., Rheo-FTIR [1], Rheo-TD-NMR [2], and Rheo-DES [3]. In the last years, the method of Rheo-IR was developed and subsequently improved. The recent developments and improvements in the combined technique Rheo-IR, and example measurements, that show the correlation between molecular and macroscopic level will be presented in this contribution.

Keywords: Combined Methods, Rheo-IR, Rheology, Infrared spectroscopy

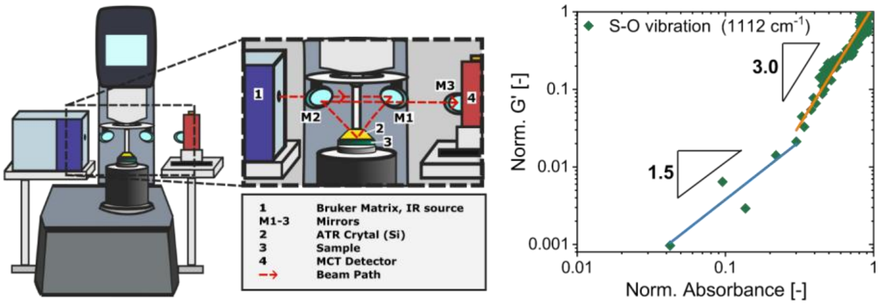

Figure 1. *left: Rheo-Combined-IR-Spectroscopy setup; right: correlated rheological and IR data.*

Acknowledgements: WI 1911/25-1, project number 386871659, DFG priority programme 2005 "Opus Fluidum Futurum".

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Optimizing the Fabrication of Isoporous Block Copolymer Membranes by coupled Particle-based and Continuum Modelings

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Integral-asymmetric copolymer membranes represent a promising class of functional macromolecular systems with diverse potential applications, including water purification and protein separation. Their fabrication is achieved through a two-step process: (i) the controlled self-assembly of diblock copolymers upon solvent evaporation to form a cylindrical top morphology that is oriented perpendicular to the solution-gas interface. (ii) a solvent-nonsolvent exchange through immersion into a water bath, raising the polymer concentration above its glass transition, thereby freezing the matrix phase while allowing the entry of the nonsolvent through the cylindrical minority domains. Below, the nonsolvent macrophase separates from the polymer to form a macroporous substructure. Simulating this fabrication process is challenging, because it involves large length (~ μm) and time scales (~s), and several physical phenomena.

We model the process using two complementary schemes — a highly coarse-grained, particle-based model that treats the polymer chains directly [1], and a continuum model, describing the system only by its concentration fields. To exploit the accuracy of the former while retaining the efficiency of the latter, we couple the two simulations, modelling the whole system with the continuum model, which launches a particle-based model in the region of its lowest accuracy, typically where structure formation occurs. A neural network is employed to estimate the future error and guide the decision of the sub-domain. The particle-based model periodically returns the density. We efficiently perform our simulations on the JUWELS Booster at the Jülich Center for Supercomputing, with a single GPU allocated to the continuum model and several other GPUs for the computationally intense particle-based model. This approach yields a tenfold increase in computational efficiency compared to pure particle-based simulations, enabling us to investigate solution film depths exceeding 100 times the polymer end-to-end distance. Finally, our simulations delineate a process window for successfully fabricating of integral-asymmetric copolymer membranes.

Keywords: polymer membranes, simulation, self-assembly, diblock copolymers

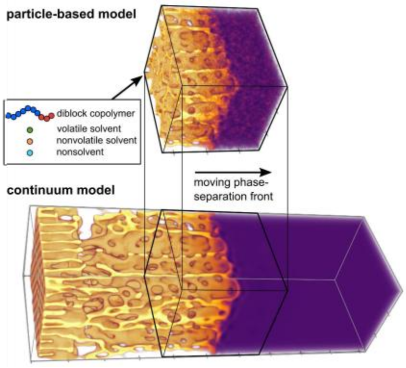

Figure 1. *Coupled simulation of the membrane fabrication process.*

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Tuesday 30th September 2025

G. Glasses, Granular, Jamming

(Room 4)

Self-organization and emergence of memory in a cyclically driven model of amorphous plasticity

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The mechanical behavior of disordered materials, such as dense suspensions, glasses, and granular materials, depends on their thermal and mechanical history. Under periodic driving, these materials can evolve into states that encode a memory of their annealing. Such memory effects have been observed experimentally in systems ranging from sheared non-Brownian suspensions to crumpled elastic sheets and in atomistic simulations. Here, we show that a quenched mesoscopic elasto-plastic model of a sheared amorphous solid reproduces the phenomena of self-organization and memory formation under mechanical annealing. We analyze sample-to-sample fluctuations under read-out protocols and demonstrate their connection to the irreversibility transition. Our model allows us to understand in detail the mechanical processes underlying memory formation. We find that annealing by cyclic shear leads to the self-organization of plasticity, which can be characterized by a density of local mechanical stress thresholds. These thresholds exhibit anisotropy, depending on their alignment with the driving direction. The interplay between these thresholds dictates how the driving history — particularly its direction and amplitude — is imprinted into the material's local structure. We develop read-out protocols capable of accessing both the amplitude and the direction of the mechanical training. Our findings can be understood within the framework of return point memory which emerges as a result of mechanical annealing. Building on this, we develop a Preisachlike model of directional memory that describes well our numerical results. We conclude with a discussion of similarities of the evolution of plasticity under mechanical annealing and adaptive evolution in changing environments.

Keywords: memory, self-organization, elasto-plastic model,

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Generating ultra-stable glasses by homogenizing the local virial stress

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Experimental realization of ultra-stable glasses (UG), employed in technological applications like OLED displays and amorphous pharmaceuticals, has sparked renewed interest in algorithms capable of generating glasses with enhanced properties. In parallel, the algorithmic preparation of ultrastable glasses has considerably expanded our understanding of the glassy state.

In this work, we present a new protocol for UG preparation (see Figure 1) in a model colloidal glass, which iteratively modifies particle diameters to reduce local virial stress fluctuations, effectively homogenizing the local mechanical environment of individual particles [1]. We apply the algorithm to an additive Lennard-Jones mixture and show that, compared to the states obtained via thermal annealing, virial homogenized glasses (VHG) are characterized by a considerable increase in both kinetic stability and the number of locally favored structures, and melt during heating ramps via an accumulation of localized events. Our results show that microscopic mechanical homogeneity, a widely applicable concept, can give rise to ultra-stability.

We then ask whether ultra-stable glasses produced by other methods also exhibit the hallmarks of virial homogeneity. By applying the swap algorithm to liquids and glasses at a variety of temperatures, we find that the inherent structures of equilibrated glasses at lower temperatures display significantly narrower distribution in local virial stress. This shows that the generation of ultra-stable glasses via swap equilibration spontaneously induces homogeneity in local stress. In conclusion, we suggest that not only can non-equilibrium reduction of the second moment of local stress through virial homogenization leads to ultra-stable glasses, but ultra-stable colloidal glasses also exhibit the key hallmarks of VHG states.

Keywords: ultra-stable glasses, virial stress, molecular dynamics simulations

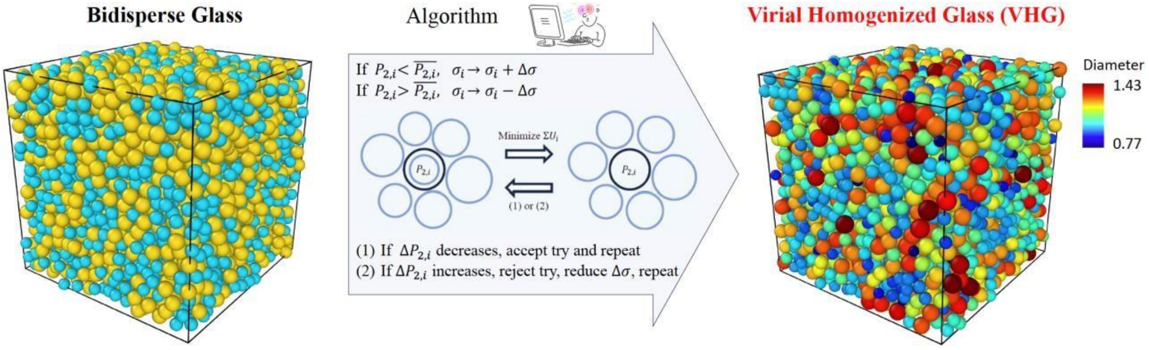

Figure 1. *Application of the VHG algorithm to a bi-disperse glass to obtain an ultra-stable glass. The algorithm iteratively modifies particle diameters to reduce local virial stress fluctuations effectively homogenizing the local mechanical environment of individual particles.*

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Kovacs-like memory effect in a sheared colloidal glass: role of non-affine flows

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Memory effects reflect a system's ability to encode, retain, and retrieve information about its past. These effects, inherently out-of-equilibrium phenomena, provide valuable insights into the complex structural and dynamical behavior of a system. The Kovacs effect is one such memory effect traditionally associated with thermal history. While studies have extended Kovacs-like memory to mechanical perturbations such as compression-decompression, its presence under volumeconserving perturbations like shear remains unexplored.

In this work, combining experiments, simulations, and linear response theory, we demonstrate the Kovacs-like memory effect in a sheared colloidal glass. Furthermore, we investigate the influence of non-linear perturbations and establish a correlation between deviations from linear response predictions and microscopic non-affine flows arising from large deformations. Our study not only extends the domain of Kovacs-like memory effects to volume-conserving mechanical perturbations but also highlights the importance of the nature of underlying microscopic flows in controlling the bulk stress relaxation, affecting the Kovacs-like memory effect in amorphous materials.

Keywords: Memory, Kovacs effect, Colloidal glass, Shear, Nonaffinity

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Supercritical density fluctuations and structural heterogeneity in supercooled water-glycerol microdroplets

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Recent experiments and theoretical studies strongly suggest that water undergoes a liquid-liquid phase transition (LLPT) in the supercooled regime. However, how this behavior influences aqueous solutions remains an open question. In this study [1], we combine femtosecond small- and wide-angle X-ray scattering (SAXS/WAXS) with molecular dynamics (MD) simulations to investigate supercooled glycerol–water microdroplets at dilute conditions (χ_g = 3.2% glycerol mole fraction) over a wide temperature range (229.3–295 K). To access the deep supercool regime, we utilize rapid evaporative cooling of microdroplets. We find that, both the isothermal compressibility (κ_T) and correlation length (ξ) of the solution increase anomalously upon cooling, following a power-law behavior, and the addition of glycerol suppresses these density fluctuations and shifts the κ_T-maximum of water from ~230 K to ~223 K. While this shift suggests the system remains in the supercritical regime, structural markers, such as the local order and the existence (and temperature crossover) of High-density-liquid (HDL) / Low-density-liquid (LDL) populations, remain similar to pure water. This indicates that the hypothesized framework of a second critical point in water, extends to dilute aqueous solutions, with glycerol modifying the temperature response of the system. We therefore suggest that, by modulating collective fluctuations, glycerol contributes to cryoprotection, potentially delaying nucleation and ice formation. This work provides a framework for designing optimized cryoprotectant mixtures and could inform future developments in cryopreservation, especially for complex biological systems where avoiding ice nucleation is critical.

Keywords: supercooled water, glycerol, cryoprotectants, LLCP, Widom line

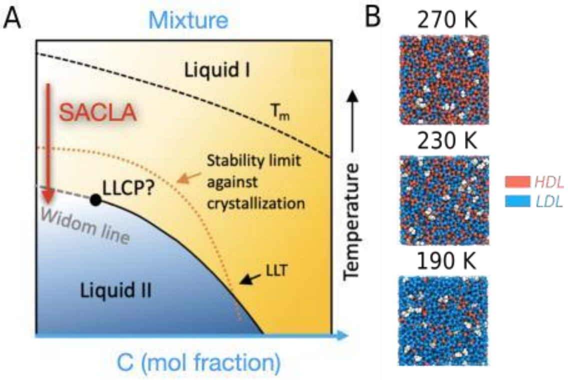

Figure 1. A) *Schematic representation of the Temperature – concentration phase diagram of the solution. The downward red arrow indicates the range of temperatures that were probed in this study.* ***B)*** *Snapshots of the MD simulation box of the solution, with colored water molecules, according to their local structure (LDL, HDL).*

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Charged Rod-Glasses in non-Equilibrium Shear Flow Response

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The equilibrium phase behaviour [1-3] are presented for the concentrated suspension of bacteriophage fd, DNA-viruses charged DNA-viruses, at sufficiently low ionic strengths (below 1 mM Tris/HCl buffer), which is a good model system for highly charged colloidal rods, exhibiting the phase transitions; from the nematic-to-chiral nematic and other hierarchical chiral-mesophases (Xpattern and helical domains) to the glass states, in an increase of the rod-concentration [4-5]. In this talk, experiments on both equilibrium and the field-induced phase transition, as well as sheer response of the glass state in flow will be discussed. The (structural) glass transition occurs well within the full chiral-nematic state, where the particle dynamics and the orientation texture dynamics are simultaneously arrested, at the same concentration [3-5]. The glass is also found to exhibit several types of non-uniform flow profiles, depending on the externally applied shear rate: At low shear rates plug flow is observed and at intermediate shear rates gradient-banded flow profiles are found [4, 5]. At high shear rates the glass is melted, leading to a linear flow profile. Finally, as one of interesting findings for chiral-mesophases, is a "chiral-glass", driven by the replica symmetry breaking (RSB), determined by both real- and Fourier-space [6], kept between the two "replicas" of larger chiral-nematic domain (at a lower concentration) and the "helical-domains" (at a higher concentration) of charged DNA-rods [7]. As will be shown, there is a subtle interplay between the stress originating from inter-particle interactions within the domains and the texture stress due to inter-domain interactions.

Keywords: Rod-glasses, charged colloidal rods, DNA-viruses, Chiral-mesophases, Chiral-glass

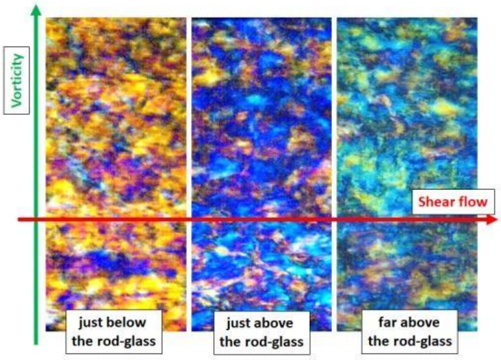

Figure 1. *Typical orientational textures of rod-glasses in simple shear-flow (vorticity-flow plane)*

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Rheology of Curved Rods and Applications in Biological Systems

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Dense suspensions are a broad class of out-of-equilibrium systems that often display interesting macroscopic behaviour under flow. The rich physics observed for suspensions of spheres can be expanded to particles of more complex geometries. This work applies concepts from dry granular physics to model the rheology of suspensions of curved rods. The curvature-dependent jamming volume fraction, $\phi_{!}$, is investigated in both monodisperse and polydisperse systems, whereby mixtures of morphologies provide insight into blood flow blockages that occur in sickle cell anemia patients. We try to understand such mechanisms of jamming by quantifying structural properties such as co-ordinate number, alignment and interlocking.

Keywords: Rod-like rheology, polydispersity, jamming transitions, orientational order

Criticality of the viscous to inertial transition near jamming in non-Brownian suspensions

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In this work, a Discrete Element Method (DEM) is used to explore the viscous to inertial shear thickening transition of dense frictionless non-Brownian suspensions close to jamming. This transition is characterized by a change in the steady state rheology of a suspension with increasing shear rate from a regime of constant viscosity at low shear rates to a regime where the viscosity varies linearly with the shear rate. The numerical simulations show that the characteristic shear rate associated with this transition depends sensitively on the volume fraction of the suspension and that it goes to zero as we approach the jamming volume fraction for the system. A scaling framework is formulated that allows for a collapse of the rheological data associated with the viscous to inertial transition and showcases the criticality of this transition at jamming. This criticality is further shown to be associated with a growing length scale of the microstructure that diverges at jamming.

Modelling the flow-induced anisotropy of the mechanical response of concentrated suspensions

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Suspensions, which exhibit complex behaviors such as shear thickening, thinning, and jamming, are prevalent in nature and industry. However, predicting the mechanical properties of concentrated suspensions, and especially transient ones, remains a significant challenge, impacting product quality and process efficiency. In this study, we focus on developing a robust theoretical framework to explain how flow history governs the anisotropy of mechanical responses in suspensions of hard particles under unsteady flow conditions. Our starting point is the Gillissen-Wilson constitutive model [1], which we confront to DEM simulation data of the microstructure and stress responses during steady shear, shear reversal, and shear rotations [2-3], where the shear axis is rotated by a specific angle. We use our measurements of the distinct contributions of hydrodynamic forces and particle contacts to the stress response to inform improvements to the Gillissen-Wilson model.

Keywords: Dense Suspensions, Gillissen-Wilson, Theoretical Model.

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New Insights into PNIPAM Microgel Behaviour: The Role of Crosslinker Density and Particle Softness

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Microgels, a notable class of soft colloids, are composed of particles formed by crosslinked polymer networks. They have attracted significant attention due to their unique properties including deformability, elasticity, and potential interpenetrability. Additionally, their responsiveness to environmental stimuli makes them attractive for a wide range of applications.

In this study, aqueous suspensions of microgels based on the thermo-sensitive polymer poly(N-isopropylacrylamide) (PNIPAM) were synthesized and systematically investigated, to evaluate the effect of varying crosslinker content.

Changes in crosslinker concentration affects the softness of the microgel particles, thereby influencing their structural, dynamical, rheological, and thermodynamic properties.

Although the influence of crosslinking density on the properties of PNIPAM microgels has been thoroughly investigated, [1-7] here further insights are presented through a comprehensive approach, employing multiple experimental techniques to explore the role of crosslinker density at different concentrations and its impact on the overall behaviour of PNIPAM microgels.

Keywords: microgels, softness, rheology

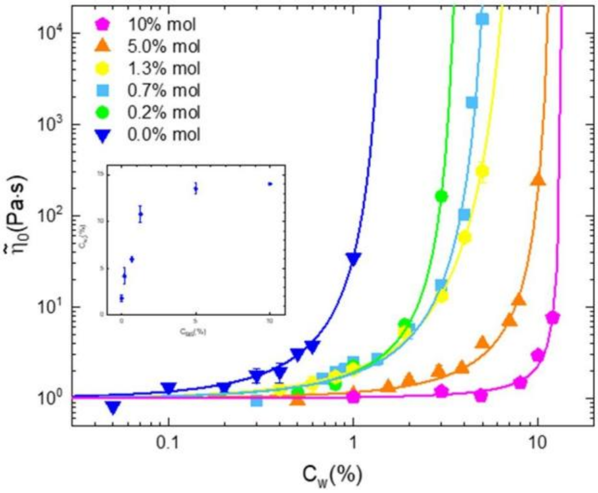

Figure 1. *Normalized viscosity as a function of microgel concentration at different crosslinker densities in the range 010% mol. Inset: glass transition concentrations as a function of crosslinker concentrations (C_{BIS})*

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Slow out of equilibrium dynamics in soft colloidal glasses: the role of gravity

Alessandro Martinelli [1], *Stefano Buzzaccaro* [2], *Rajam Elancheliyan* [3], *Domenico Truzzolillo* [1], *Juliette Behra* [1], *Niel Segers* [4], *Erik Leussink* [4], *Roberto Piazza* [2], *and Luca Cipelletti* [1,5]

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Despite gravitational forces are rarely relevant at the single colloidal particle scale, they do play a crucial role when colloids assemble to form large structures. In fact, gravitational stresses may be transmitted and accumulated over macroscopic distances, strongly changing the spontaneous dynamical properties of the system at study.

In this talk, I will discuss the capabilities of Colloidal Solids (COLIS), a state-of-the-art light scattering setup developed for experiments in microgravity onboard the International Space Station (ISS). This innovative setup allows for probing the structure and dynamics of soft matter systems on a wide range of length scales, from a few nm to tens of microns, and on time scales from 100 ns to tens of hours [1]. The setup includes different state-of-the art experimental approaches, ranging from multi-angle photon correlation imaging, small angle static light scattering to optical manipulation of thermosensitive samples through an auxiliary near-infrared laser beam.

I will focus here on suspensions of ultra-low cross-linked PNIPAM microgels, in which glass transition can be induced with temperature variations as well as number density variations. I will show how these soft systems can be driven in the glassy state and how they can be perturbed with local temperature increases induced by the near-infrared laser, leading to non-diffusive microscopic relaxations characterized by compressed density correlation functions and reminiscent of the behavior of soft solids under oscillating shear [1].

Finally, I will report the current progress of the experimental campaign in microgravity for the PNIPAM microgel glasses.

Keywords: microgravity, dynamic light scattering, soft glasses

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Hollow microgels: From single particle characterisation to bulk behaviour

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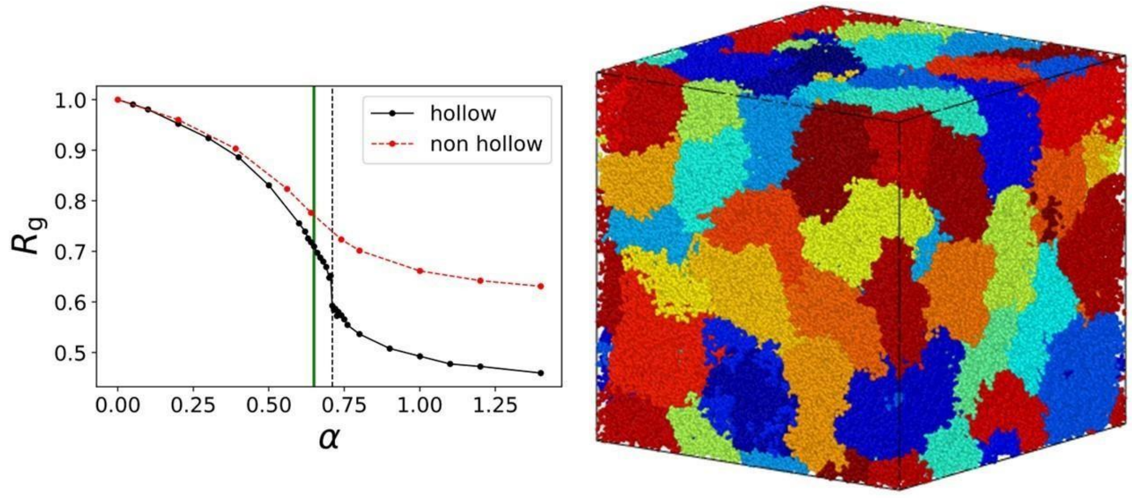
Hollow microgels, composed of a pNIPAM polymer network with a central cavity, offer tunable softness and the potential of encapsulation. Using molecular dynamics simulations, we characterise their swelling behaviour across the Volume Phase Transition (VPT) by varying crosslinker concentration, shell thickness, and size. We identify a discontinuity in the radius of gyration R_g as a function of temperature, shown in Figure 1 (a) and linked to cavity filling when a certain balance of shell stiffness and thermoresponsiveness is achieved. Validation against experimental form factors confirms our model, and we establish a suitable and stable hollow microgel of moderate monomer number as candidates for computationally feasible bulk simulations. In our initial bulk simulations, we observed indications of so-called buckling—defined as the transition from spherical to bowlshaped under asymmetric collapse due to external stress, in our case high densities. This is evident from some sickle-shaped microgels in the snapshot of Figure 1 (b). Additionally, the radius of gyration and asphericity distributions of the bulk deviate from a Gaussian curve, with a second maximum emerging, potentially linked to preferred shapes. Overall, these findings provide valuable insights into the swelling properties, buckling behaviour, and shape preferences of hollow microgels, advancing their control for practical applications.

Keywords: hollow microgels, Molecular dynamics simulations, swelling behaviour, bulk, buckling



(a) (b)

Figure 1. *(a) Characteristic swelling curve, measured via radius of gyration R_g, of a hollow microgel compared to a non-hollow microgel. The vertical green line marks the VPT while the black dashed line refers to the cavity filling. (b) High-density bulk simulations of identical hollow microgels with first signs of buckling. Some of the deformable hollow microgels are found in a bucked state to efficiently occupy the available space.*

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Structural Signatures of Mechanical and Thermal Activation in Amorphous Matter

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Structural relaxation in supercooled fluids is spatially and dynamically heterogeneous, with regions of fast particles coexisting near slow ones when the material evolves through spontaneous thermal activation. In sheared glasses at low temperature, where the activation is purely mechanical, deformation proceeds instead via localized shear transformations. Substantial efforts have been directed towards establishing whether such local dynamics also has a local structural origin [1]. We explore the structural signatures of local excitations in glassy liquids and solids with the atomic cluster expansion (ACE), a universal and complete linear basis of descriptors of the atomic environment [2]. Body-ordered linear classifiers are constructed that distinguish between active and inactive particles in a polymer glass and two different types of binary mixtures, in which structural relaxation occurs either through spontaneous thermal activation or by simple shear. We find that in binary mixtures, maximum prediction accuracy is already achieved with very few twobody correlations, while a polymer glass requires both two-and three-body correlations. Trends are robust across both activation mechanisms. Dimensionality reduction is then employed to construct a minimal set of descriptors, and opportunities to improve the predictions via multi-layer neural network architectures are explored.

Keywords: glassy dynamics, dynamical heterogeneity, shear transformation, atomic cluster expansion

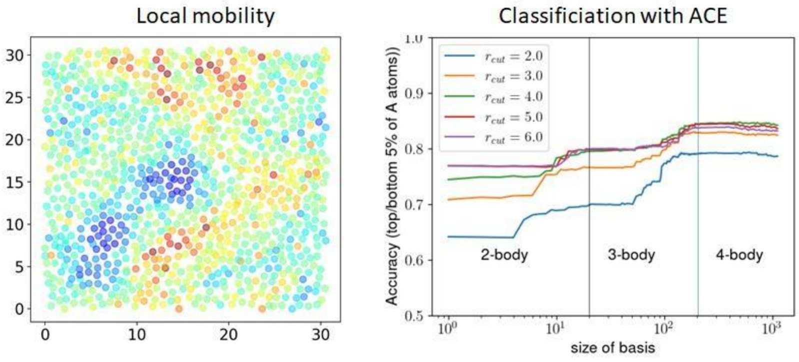

Figure 1. *Left: Dynamical heterogeneity in a polymer glass near the glass transition. Right: classification of local mobility with the atomic cluster expansion*

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On the local alignment and anisotropy of stresses in disordered granular media

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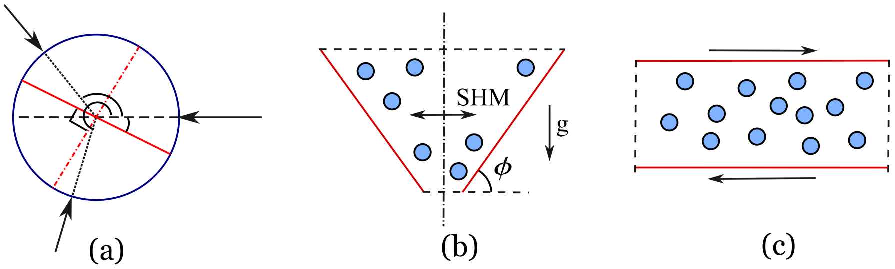
Characterizing the relation between local stress states and bulk mechanical properties is a key challenge in obtaining the statistical mechanics description of granular materials. Towards this end, we study an isolated granular cluster of 6 identical disks to identify all theoretically admissible configurations satisfying equilibrium conditions. For each of these configurations, we determine the associated contact forces, and subsequently calculate the particle-level volume-averaged Cauchy stress via the force-moment tensor, as shown in Figure 1(a). The corresponding eigenvalues and eigenvectors allow us to study the stress anisotropy, defined as the ratio of the shear stress to the hydrostatic stress, within each disk, and the degree of misalignment between the particle-level stress transmission directions for the contacting particles. We then impose physically-motivated pairwise constraints on the geometric arrangement and the force solutions and focus on the special case of non-cohesive hard disks.

Furthermore, we perform DEM simulations of a 2-dimensional hopper—with varying slant angle (ϕ), filled with slightly polydisperse particles evacuating under the influence of gravity (refer to Figure 1(b)). We employ the recursive force-chain algorithm proposed in [1] over these particles immersed in the bulk and observe consistent trends in the probability distribution of anisotropy, as well as the principal stress alignment. The key signatures persist even when the hopper is subjected to a simple harmonic motion orthogonal to the flow direction, or when switching to an entirely different system—plane shear (shown in 1(c)). We compare the statistics from these simulations to those from the isolated cluster case and show that the primitive model already possesses the germ for the trends observed for the bulk. We finally provide a range for the critical chain parameter angle α, hitherto set arbitrarily [1-2], to sample force-links while constructing force-chains.

Keywords: force chains, principal stresses, DEM simulation



(a) (b) (c)

Figure 1. *(a) principal stresses (σ_1, σ_2) in a particle in the isolated cluster model, (b) hopper and, (c) plane shear setup used in the Discrete Element Method simulations*

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Microscopic structure and dynamics of shear thinning suspension of polydisperse repulsive vesicles

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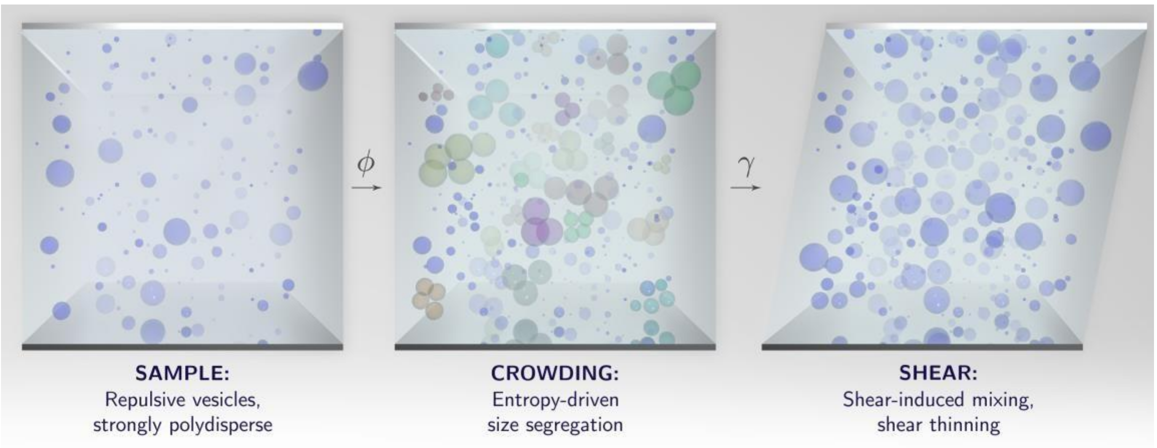
We investigate the rheology, microscopic structure, and dynamics of an industrially relevant dispersion made of charged vesicles, from dilute to concentrated conditions. We find that these suspensions exhibit a shear-thinning behavior at relatively low concentrations. At the microscale, this corresponds to a well-defined transition in both the structure, marked by the appearance of a peak in the static structure factor, and the dynamics, which slow down and develop a two-step decay in the correlation functions. This low-concentration transition is particularly surprising in light of experiments showing that for surfactant vesicles of similar composition the interactions should be purely repulsive. This leads us to propose that the observed structural and dynamic transition could arise, as an entropic effect, from the large sample polydispersity coupled to crowding. The shearthinning behavior is thus interpreted as the nonlinear response of this transient structure to the imposed flow. Our work suggests that similar effects might be a generic feature of dense, highly polydisperse charged suspensions.

Keywords: shear thinning, polydispersity, multiscale characterization.



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Effects of particle angularity on the self-organisation of intergranular cells

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Voids surrounded by particles in contact ("cells") are the most basic organizable structure in granular media. Recent studies of two-dimensional packings have shown that cells and cell properties selforganize during quasi-static processes independent of the processes involved [1]. However, due to the complexity of simulating particle shape, the majority of preceding work was performed for packings of round particles, for which higher particle mobility reduces the overall stability of granular aggregates. While the effect of shape and its combined influence with friction on the bulk properties of aggregates has received some attention [2], little is yet understood about their influence on the cell microstructure. In this work we systematically explore the effects of particle angularity and friction on different indicators of cell self-organisation by means of Discrete Element Simulations of isotropic biaxial compression tests.

In particular, we show that, while the cell orientation always aligns with applied stresses, the quality of the collapse of the conditional probability of the cell stress ratio h onto a master form for different friction coefficients depends on the angularity of the particles.

Keywords: Non-spherical Particles, Friction, Stress-Structure Self-Organization

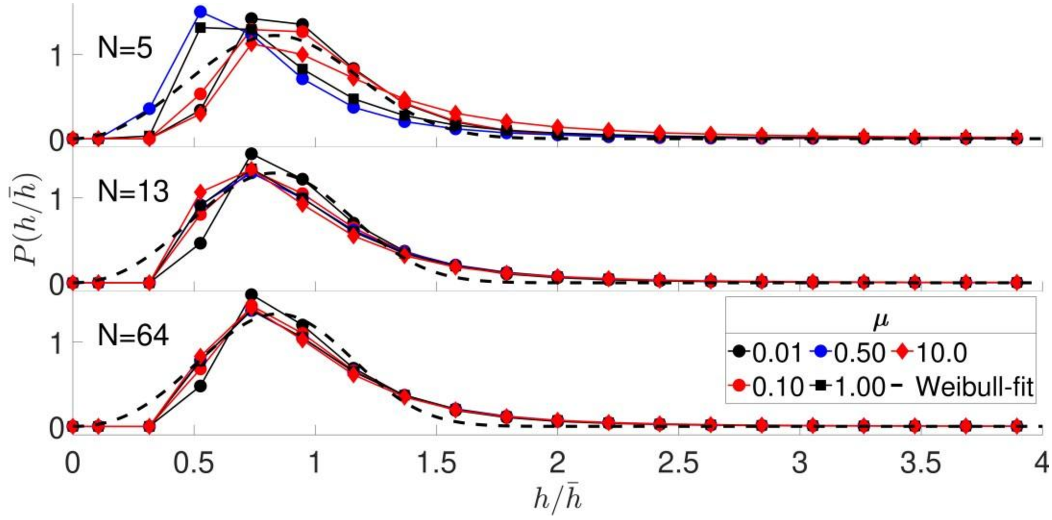

Figure 1. *As the particles become more angular (smaller N) the conditional probabilities of the cell stress ratio, h, increasingly deviate from an optimal Weibull-fit.*

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Self-Assembly of Charged Granular Matter under Acoustic Levitation

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Granular matter self-assembly underpins the formation of complex structures in both natural and engineered systems. Acoustic levitation provides a powerful tool for studying such processes by eliminating the effects of gravity and container walls, allowing granular self-assembly to occur under well-controlled, boundary-free conditions. We have developed a technique that combines acoustic levitation with controlled electrostatic charging to assemble, transform, and activate complex many-particle structures.

In an acoustic field alone, particles aggregate into two-dimensional, densely packed ("compact") configurations due to attractive in-plane forces established by acoustic scattering. However, introducing long-range electrostatic repulsion allows some particles to overcome these attractions, leading to the formation of "expanded" and "semi-expanded" structures, where interparticle separation distances reach a few times the particle diameter. For small particle numbers, electrostatic forces tend to dominate, producing fully expanded configurations. For larger ensembles, the interplay between short-range attractive acoustic forces and long-range repulsive electrostatic forces typically results in semi-expanded structures, where a central compact core is surrounded by "satellite" particles—a configuration unattainable with either interaction alone. We observe and investigate active rotations, synchronized oscillations, and coupled motions between the core and satellite particles. Our system represents a novel platform for studying selfassembly driven by competing short- and long-range forces, revealing rich collective dynamics and structural transitions inaccessible in conventional systems.

Keywords: acoustic levitation, self assembly, granular matter

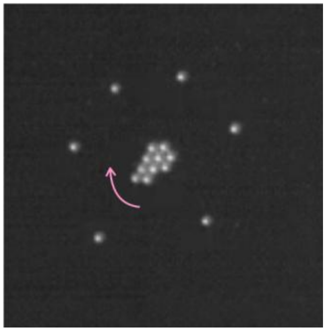

Figure 1. *Bottom view of a semi-expanded structure consisting of charged Ag coated PMMA spheres (250 micron in diameter). Clockwise rotation of the central cluster triggers coupled oscillations of "satellite" particles.*

Topology of Knitting: Marginal Constraints and Knittability

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Knitted textiles exhibit unique topological and mechanical properties, distinct from woven and other fabrics. A key feature of knitting is the topological constraint that yarn ends remain fixed at infinity during the fabrication process. This constraint suggests a fundamental classification of textiles: those can be knitted and cannot (Fig.1 (a)). However, a systematic classification based on knittability has remained elusive, despite previous attempts [1].

Here, we define knittability in terms of knot theory and clarify the stability of the textiles from a topological viewpoint [2]. We construct a mapping from a given textile structure to a corresponding knot and introduce a line defect into this knot. A textile is knittable if and only if the defect allows the knot to be deformed into a trivial one. This interpretation provides a framework for understanding knitting as a marginally constrained textile, where partial destruction causes the whole collapse. Knitting is a textile at the edge of topological stability.

Furthermore, we show that defect propagation enables an efficient method to determine knittability and unlocks new design possibilities. By controlling defect copy, we demonstrate the feasibility of programmable textile properties, such as robustness against breakdown, and mechanical memory. These findings establish a new link between topology and soft matter physics, offering a foundation for the next generation of functional textiles.

Keywords: Topology, knitting, fracture

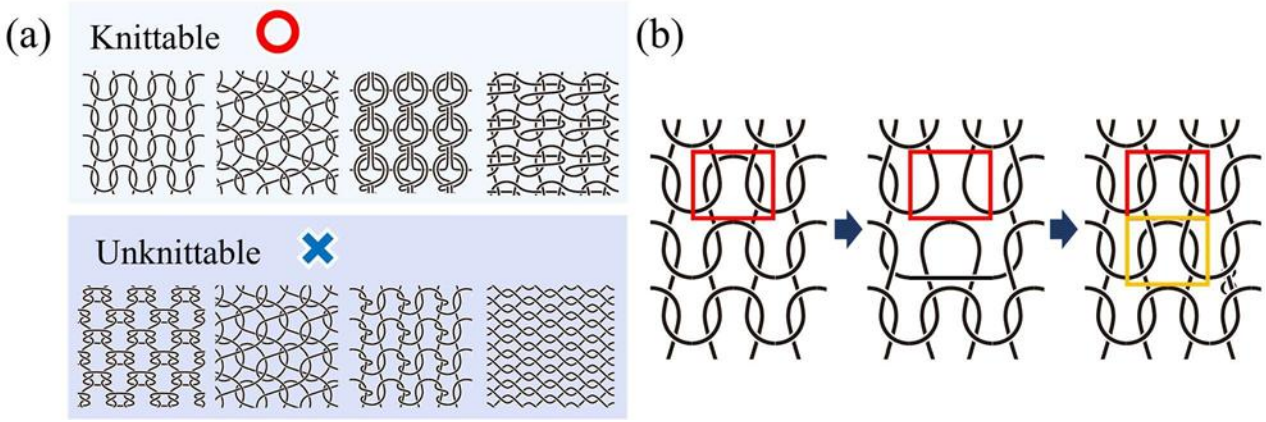

Figure 1. *(a) Examples of textiles which can be made by knitting and not. (b) An example of the defect copy only by the continuous deformation in the knittable textile.*

Acknowledgements: This research was funded by the Japan Society for the Promotion of Science (JSPS) KAKENHI [grant nos. 23KJ0753].

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Wednesday 1st October 2025

A. Active matter

(Room 1)

Swimming *E. coli* power the rotation of symmetric discs

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Suspensions of swimming *E. coli* bacteria are a non-equilibrium bath for objects immersed in them. They agitate objects more than a thermal bath and power the rotation of gears, provided they are *asymmetric*, a result of the collisions of E. Coli with the rotors boundaries [1, 2].
In contrast with previous results, here we show the persistent rotation of *symmetric* objects in a bacterial bath of swimming E. Coli. Combining experiments and hydrodynamic modeling, we elucidate the mechanism as contactless and of hydrodynamic origin. The counter-rotation of the flagella and the bacterium body exerts a torque dipole inducing the observed rotation. We notably demonstrate quantitative agreement between our experiments and the hydrodynamic model. Our findings provide further fundamental insights into bacterial hydrodynamics and open avenues for the development of autonomous, self-powered micro-rotors for the study of chiral fluids

Keywords: fluid dynamics, bacterial flagellar motors, *E.coli*, hybrid micromachines

Figure 1. *It must not exceed the limit of 17cm wide. Do not wrap the text around any of the graphics.*

Acknowledgements: JP, DG acknowledges support from ERC grant (VULCAN, 101086998)

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Memory effects for the trapping of the phototactic micro-alga *Chlamydomonas reinhardtii* within light patterns

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Chlamydomonas reinhardtii cells have the ability to orient themselves in light fields, a property called phototaxis. These cells can perform both positive and negative phototaxis, i.e. migrating towards the regions of higher or lower intensity respectively. The conditions for the switching between these two opposite behaviors is still poorly understood. Recently it has been shown that the switch is accompanied by short-term memory effects [1].

In this talk I will show that this short-term memory can be exploited to trap cells within light patterns, such as a ring-shaped beam (Fig. 1). Thanks to a detailed quantification of the motility of the cells within the different regions of the light pattern, we were able to build a simple model for their phototactic behavior that recapitulates very well the trapping phenomenon. Our results provide insights towards the fine control of the localization or rectification of active phototactic particles, whether they are biological or synthetic.

Keywords: phototaxis, memory, trapping, Chlamydomonas

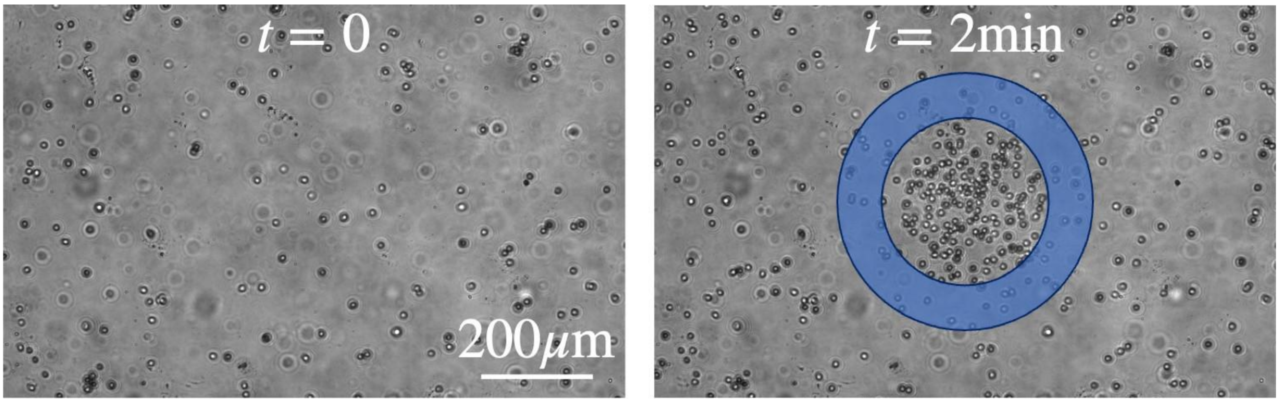

Figure 1. *When confined to a quasi-2D chamber (20μm-thick) and illuminated by a ring-shaped beam, Chlamydomonas cells quickly get trapped and accumulate inside the ring. We rationalized this phenomenon by studying the modulation of the motility of the cells within the different regions of the illumination pattern, and showing that it is the consequence of a memory effect in the switching between positive and negative phototaxis.*

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Bacterial motility during the early-stage of interaction with surfaces functionalized with nano-antimicrobics

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Understanding the bioactivity mechanisms of antimicrobial coatings is crucial for the development of safer materials, limiting the development of antimicrobial resistance through a correct control of dose-effect relations. Therefore, the effects of the microbe-surface interactions on bacterial motility need to be characterized in detail at different stages. In this work we investigated the motility of bacteria in the early stage of interaction with ZnO-based bioactive surfaces. Inorganic antimicrobials were embedded into polyethylene oxide, polylactic acid and poly-vinyl-methyl-ketone to produce nanocomposite coatings providing different release of Zn^{2+} ions (i.e. tuneable bioactivity). To establish an analytical dose-effect correlation, the influence of Zn^{2+} release on the motility of *Bacillus subtilis* was evaluated using particle tracking analysis applied to confocal microscopy experiments [1,2]. The average mean squared displacements (MSDs) revealed that the run-and-tumble dynamics of *B. Subtilis* quickly turn into diffusive and sub-diffusive motion under the effect of increasing Zn^{2+} release (Fig.1), with an associated broadening of the median velocity distribution and a strong reduction of its average value. Detailed analysis of trajectories shows that the population of actively swimming bacteria is strongly depressed at all Zn^{2+} ions releases, while increasing release the population of diffusing bacteria is progressively decreasing in favour of the sub-diffusive population (Fig.1). Our results thus show that in the early stage of interaction the antimicrobial action is biostatic: *B. Subtilis* motility is generally suppressed by the release of Zn^{2+} ions. However, bacteria are still alive and mobile, showing a combination of diffusive and sub-diffusive dynamics that can be tuned through the Zn^{2+} ions release. Our approach offers a new paradigm in the development of bacteriostatic vs bactericidal strategies, allowing for a precise engineering of antimicrobial coatings to achieve a desired spatio-temporal effect.

Keywords: Antimicrobial surface; bacterial motility; particle tracking; *Bacillus subtilis*

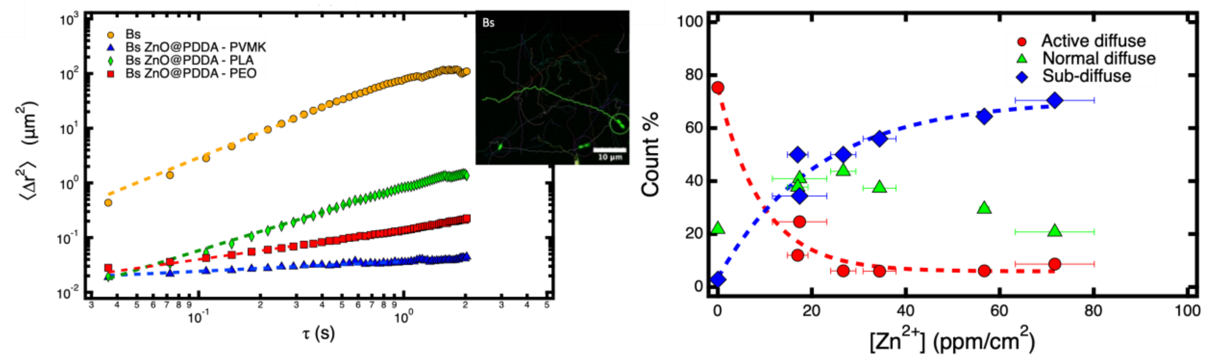

Figure 1. *Left:Mean squred displacements for bacteria in water and in contact with antimicrobial surfaces with increasing Zn^{2+} release. Inset: example of bacterial trajectory. Right: Populations of active, diffusive and sub-diffusive bacteria as a function of Zn^{2+} release.*

References

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ISMC 2025
9th International
Soft Matter Conference

Active Bacterial Baths in Droplets

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Anke Lindner[2,5]*, Teresa López-León*[3]*, Eric Clément*[2,5]*, Rodrigo Soto*[1]*, and María Luisa*
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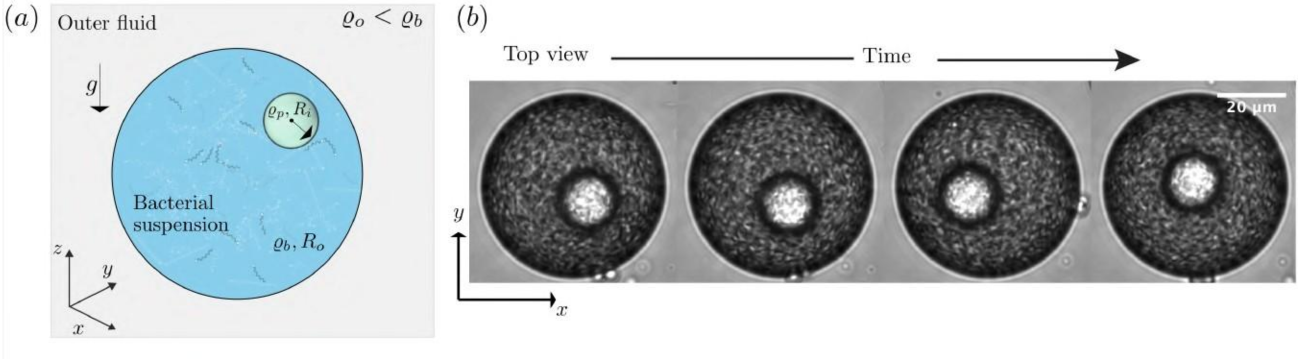
Suspensions of self-propelled objects represent a novel paradigm in colloidal science. In such "active baths", traditional concepts, such as Brownian motion, fluctuation-dissipation relations, and work extraction from heat reservoirs, must be extended beyond the conventional framework of thermal baths. Unlike thermal baths, which are characterized by a single parameter, the temperature, the fundamental descriptors of an active bath remain elusive, especially in confined environments. In this study, buoyant passive tracers are employed as generalized probes to investigate an active bath comprising motile bacteria confined within a droplet. We demonstrate that momentum transfer from the bath to the tracer can be effectively described as colored noise, characterized by temporal memory and an enhanced effective diffusivity significantly larger compared to thermal Brownian motion values. Using a stochastic analytical framework, we extract the temporal memory and diffusivity parameters that define such an active bath. Notably, the diffusivity scales linearly with bacterial concentration, modulated by a factor representing the role of confinement, expressed as the ratio of the confining radius to the probe radius. This finding, while still awaiting a complete theoretical explanation, offers new insights into the transport properties of confined active baths and paves the way for a deeper understanding of active emulsions driven by confined active matter.

Keywords: active matter-emulsions-bacterial suspension



(a) A schematic of a passive particle of radius R_i and density ρ_p confined to a spherical bacterial droplet of radius R_o and density ρ_b. The droplet is immersed in a fluid of density ρ_o. (b) A sequence of images showing the (x, y) view of the double emulsion.

Polymer dynamics in active nematic turbulence

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Polymers play a key role in many complex biomaterials in which intrinsic activity drives the system out of equilibrium. While previous studies have focused on active polymers in passive fluids or passive polymers in athermal baths, passive polymers in actively flowing liquid crystals are particularly interesting. This is because of the interplay between the broken symmetry of the anisotropic medium, nonequilibrium activity and the conformational degrees of freedom of the macromolecules. We numerically study the conformation and dynamics of individual flexible polymers coupled to the velocity field of 2D extensile active turbulence. We find diffusivity increases with activity until the onset of turbulence. The high-activity saturation is due to competition between active forcing and conformational changes. Long polymers are stretched by activity, while short polymers are compressed. While the observed extension is analogous to coil-stretch transitions of polymers in traditional inertial turbulence, the compression of short polymers is due to activity-induced curvature. This demonstrates how activity represents a pathway by which biological systems can control the steady-state structural properties of macromolecules.

Mortal vs immortal filaments: emergent properties

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Protein filaments are linear polymers vital for various cellular processes, such as cell motility, division and cell shape maintenance. To perform these processes, filaments need to actively move, which they can do via propulsion or by treadmilling. Propelled filaments have been well characterised regarding their collective behavior, and display multiple intricate dynamical states [1] which inspire applications in nanotechnology and robotics. A similar fundamental study of treadmilling filaments is missing, as the mechanism by which they mutually interact has been proposed only recently [2].

Here we compare the collective dynamics of propelled and treadmilling filaments in bulk and in confinement. We perform 2D Brownian dynamics simulations of both filament classes under various conditions. During a two-body collision, propelled filaments align by the forces they generate, while treadmilling shrink when misaligned and either align by random rotations or die. In a many-filament system, these collisions result in an ordered phase for both types, but its structure is vastly different. Propelled all collide into a single giant cluster, leaving most space empty. Treadmilling form multiple clusters with a hierarchical structure, filling the space more evenly. Because of their constant turnover, the ordered phase formed by treadmilling filaments is more robust under external mechanical perturbation. Under confinement, propelled filaments can be trapped by corners, while treadmilling die there and are reborn elsewhere.

Our results show that treadmilling results in behavior different from propulsion, for both single filaments and collectives, building a foundation for future studies in more complex settings. It also highlights the importance of birth-death processes in the healing of defects and trapped states. These findings could help us understand why the cell uses both filament types, allow us to better control physiological processes and design microscopic devices.

Keywords: treadmilling, filaments, active matter, reconstituted systems, Brownian dynamics

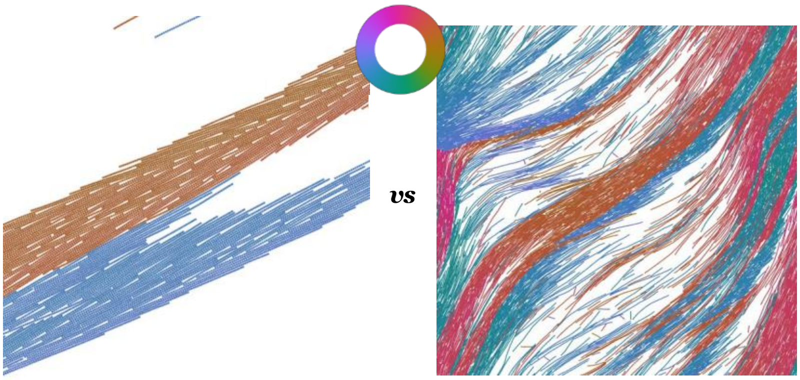

Figure 1. *Propelled filaments (left) self-organize into few linear clusters, while treadmilling (right) form multiple branched ones, filling space more evenly.*

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How do motile cells navigate soft and complex confinement?

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The motion of unicellular microorganisms in complex, anisotropic environments is ubiquitous in biology. Their natural habitats, while being quite diverse in terms of microstructure, often act as a 'soft' yet complex confinement. Remarkably, these microorganisms have developed adaptable navigation strategies that allow them to exhibit motility across a range of diverse confining environments. Here, we investigate the fundamental physical mechanisms dictating the motility of model microorganisms through different confining media of increasing complexity. Microscopic live-cell imaging (figures 1a-i and 1a-ii) of microalgal cells in polymeric media with different architectures – linear, subgranular cross-linked, and branched microgels – reveal the complex feedback mechanism between the motile microorganisms and the microstructure of the confining media. Our results (figures 1b and 1c) point towards an intricate coupling between cell motility and cooperative rearrangements within the polymeric media, which manifests as confinement-induced stress response in the microorganism. Our findings shed light on how motile micoorganisms perceive soft confinement, with implications in questions related to microbial ecology and development biology.

Keywords: soft confinement, microalgae, cell motility

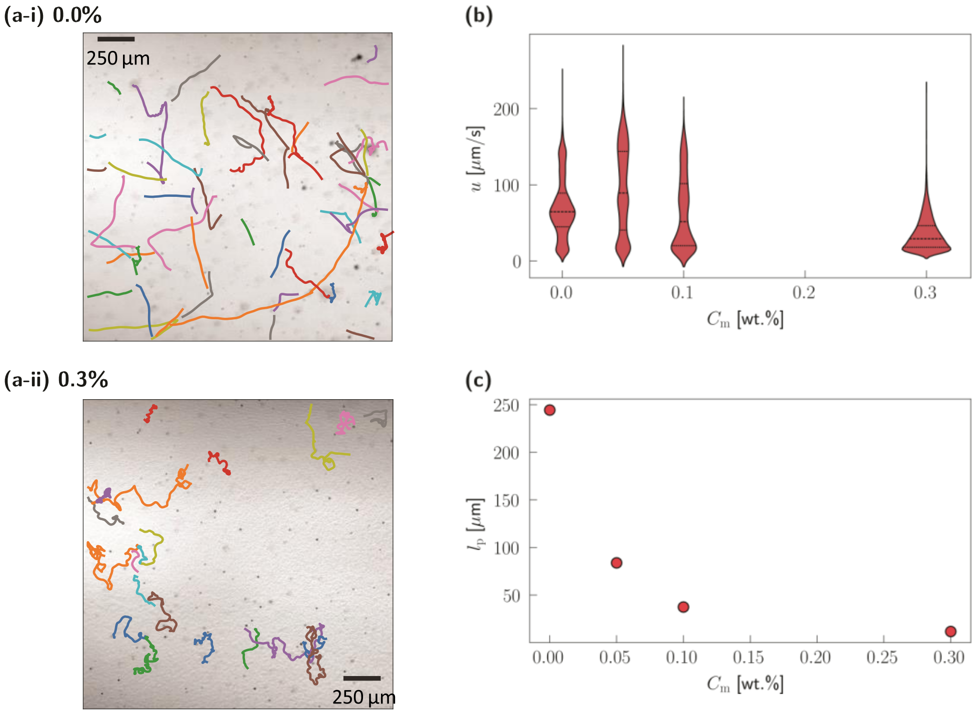

Figure 1. *Time-lapsed trajectories of motile microbial cells in a microgel dispersion of concentration (by wt.%) of (a-i) 0% and (a-ii) 0.3%. Variation of the (b) velocity and (c) persistence length of motion as a function of the microgel concentration.*

Dynamical self-assembly of active dipolar colloids into active string fluids and active networks

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Self-propelled particles with permanent magnetic dipole moments exist naturally as magnetotactic bacteria and can be engineered in active colloids and micro-robots. Yet, how the interplay between self-propulsion and anisotropic dipole–dipole interactions can be used to construct dynamically self-assembled structures in 3D remains largely unexplored. Using Brownian dynamics simulations of low-density active dipolar particles, we reveal that activity, in combination with an external field, can be used to modulate self-assembled structures with dynamically reconfigurable capabilities [1,2], akin to living matter.

Actuating dipolar particles with low to moderate active forces results in a fluid composed of tangentially driven, active polymer-like chains and rings at moderate dipolar coupling strengths. As the coupling strength increases, these structures transition into a percolated active gel with higher connectivity and more frequent configurational rearrangements [1]. As a result, the active network of aggregates exhibits greater structural and dynamical heterogeneity, accompanied by enhanced translational and rotational diffusion. A key finding is the exceptional resilience of active networks under external magnetic fields [2]. Unlike passive dipolar structures, active gels retain connectivity across a broader range of field strengths, transitioning to polarized gels only at moderate fields. Hence, we establish a design principle for engineering adaptive active materials with tunable connectivity and improved resilience through careful adjustment of dipolar interactions, external field strength, and activity level.

Keywords: active matter, dipolar active colloids, active polymers and gels

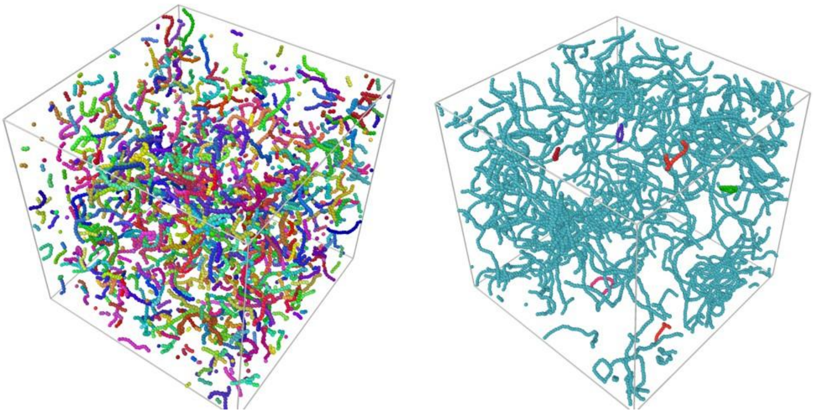

Figure 1. *Examples of active string (polymer) fluid and active gel formed by dipolar active Brownian particles.*

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Active membrane deformations of a synthetic cell-mimicking system

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Biological cells are fascinating micromachines capable of adapting their shape due to the complex interaction between a deformable membrane and the dynamic activity of the cytoskeleton. We investigate the behavior of an active synthetic cell-mimicking system (see Fig. 1) using simulations and experiments [1]. In simulations, the model consists of a fluid vesicle with a few encapsulated growing filaments. In experiments, giant vesicles contain an active cytoskeletal network composed of microtubules, crosslinkers, and molecular motors. These active vesicles show strong shape fluctuations reminiscent of shape changes of biological cells. We analyze membrane fluctuations and show how the intricate coupling between soft confinement and internal active forces results in fluctuation spectra with distinct spatial and temporal scales, differing significantly from those of passive vesicles. Simulations demonstrate the universality of this behavior, quantifying the impact of correlated activity on the dynamics of membrane deformations. This model makes a step toward quantitative description of shape-morphing artificial and living systems.

Keywords: active vesicle, membrane deformation, microtubule network, growing filaments, dynamic triangulation membrane model

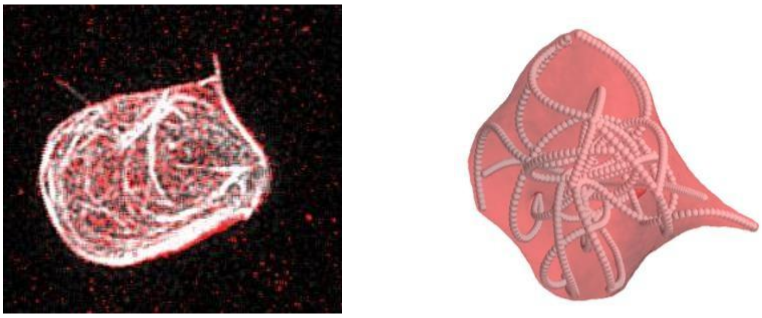

Figure 1. *(left) Confocal projection of a GUV (membrane in red) containing an active microtubule network (white). The GUV deforms and changes its shape. (right) Simulation of this active system, consisting of a vesicle and several semi-flexible filaments that grow and shrink.*

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Microbial bioconvection mitigates nutrient limitation via enhanced active flows

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Warming climate, together with frequent surface runoffs, has vastly intensified the incidence of harmful algal blooms (HABs) over the recent decades. Motile, gravitactic microplankton species drive some of the most resilient HABs, despite severe resource limitations – both in nutrient and light availability – presented by the bloom conditions. While motility confers competitive advantage to microplankton through the diel vertical migration (DVM), strong density stratifications constraints nutrient fluxes, limiting their ability to migrate across density interfaces, thus challenging their survival and fitness. In this study, we propose a self-organized biophysical mechanism wherein dense microbial suspensions, characteristic of bloom settings, generate persistent, active flow structures that mediate large-scale molecular transport and serve as an energy-efficient alternative to active migration via DVM. Using a bloom forming model phytoplankton, we present a mechanistic insight into the biophysical factors governing such emergent collective patterns and capture their eco-physiological implications in rendering HABs resilient event under nutrient and light-constraints. Leveraging our *Ocean-In-Lab* platform, together with particle tracking velocimetry and particle image velocimetry, we demonstrate that phenotypic trade-offs among cells can influence spatio-temporal self-organization, facilitating efficient molecular and micro-cargo transport. Our results indicate that active transport driven by microbial self-organization in stratified settings, significantly enhances vertical mixing, weakening density barriers, thereby facilitating nutrient redistribution.

Keywords: Bioconvection, Gravitaxis, Active transport, Stratification, Physiology

Emergence of a vortex lattice in anisotropic active flow under confinement

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We assemble a biomimetic active material from microscopic components like cells' filaments and protein motors that consume energy and generate continuous motion. Such active systems are capable of self-organization at different length and time scales, often exhibiting turbulent flows and the emergence of long-range orientational order, which is a characteristic of active nematics (AN). Previously, it was demonstrated that, by bringing into contact a two-dimensional AN with an anisotropic oil that features smectic liquid-crystalline order, it is possible to transform the originally turbulent flow of the active fluid into well-aligned flows ordered by a magnetic field [1]. Alternatively, the flow of active nematic could be controlled by confining walls [2] or arrangements of obstacles [3].
In the present work we combine both approaches: well-aligned flows of AN ordered by a magnetic field were laterally confined between walls of PDMS channels. The resulting quasi-laminar flows of AN are reorganized in arrays of vortices forming a hexagonal lattice (Fig. 1). The emergence of antiferromagnetic vortex lattices is correlated with positional ordering of topological defects and the appearance of density patterns. The observed self-organization of the active flows is activity dependent and reflects the inherent properties of the aligned AN. The described system is an example of pattern formation from instabilities of AN flows and suggests potential applications in the design and control of active materials.

Keywords: active nematics, antiferromagnetic vortex lattice, self-organization

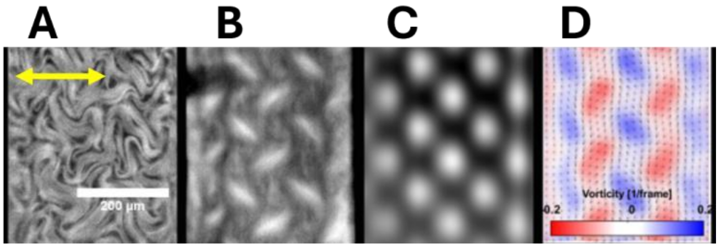

Figure 1. Patterns emerging as a result of the confinement of well aligned quasi-laminar flows of AN. (A) Instantaneous fluorescence image of AN confined in channel. (B) Time averaged fluorescence image with emerging hexagonal density pattern. (C) Band-pass filter applied to B. (D) Vortex lattice. The orientation of the magnetic field is depicted with a yellow arrow.

Acknowledgements: All authors acknowledge funding from PID2022-137713NB-C21. The presenting author also acknowledges funding from Joan Oró 2023_FI-1_00123.

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Morphological characterization of Microorganisms by Static Light Scattering

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Accurate determination of bacterial morphology and size distribution is essential for the development of theoretical and numerical models describing dense or interacting bacterial assemblies. Light scattering techniques provide a non-invasive means of bacterial characterization, enabling the measurement of complete size distributions across all stages of bacterial growth and division. This represents a significant advantage over conventional microscopy, which typically involves extensive sample preparation, manipulation, and statistical analysis, often leading to results that are less representative of native conditions.

In this study, we employed complementary light scattering methods, heterodyne near-field scattering [1] and three-dimensional cross-correlation dynamic light scattering [2], to investigate the morphology of bacteria in aqueous suspensions. These techniques yielded scattered intensity profiles across a wide range of scattering vectors for multiple bacterial strains, facilitating detailed analysis of their scattering form factors. By modeling the bacterial systems as a random ensemble of spherocylinders in suspension [3], we extracted their characteristic size distributions. Distinct scattering profiles were observed for each strain, underscoring the influence of bacterial geometry on the scattering signal. In particular, the expected intensity minima characteristic of spherocylindrical shapes were clearly resolved. The effects of polydispersity were also evident in the scattering intensity, and the applied model accurately accounted for variations in bacterial axial dimensions.

These findings underscore the effectiveness of advanced light scattering techniques in enabling rapid, non-invasive characterization of bacterial morphology. By providing detailed structural information, this approach serves as a powerful alternative to conventional microscopy. The methodologies presented here offer substantial potential for enhancing predictive models of bacterial behavior across biomedical, environmental, and industrial applications.

Keywords: Static light scattering, Microorganisms, Form factor, Morphology, Spherocylinder.

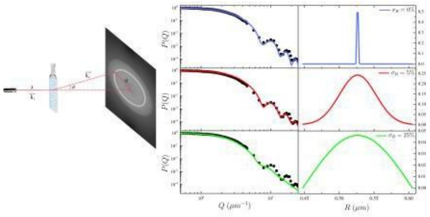

Figure 1. *Left: light scattering scheme. Middle: Form factors from E-coli, symbols (experiments) and lines (model fits). Right: size distribution from fits.*

Acknowledgements: We thank SECIHTI-Mexico for financial support (project CF-2023-I-2832).

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Wednesday 1st October 2025

B. Biological and living matter

(Room 2)

Tricks from Ticks: Phase Transitions and Adhesive Behavior of Intrinsically Disordered Tick Salivary Protein

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Ticks are ectoparasites that feed on their host for multiple days. To ensure firm attachment, they secrete a protein-rich saliva that eventually forms a solid bioadhesive, also known as the cement cone. The underlying mechanism of this liquid-to-solid transition is currently not understood. In this talk, I present our latest results on the phase transitions of a disordered glycine-rich protein (GRP) from a protein family that is abundant in the cement cone. Using microscopy, microfluidics, and mutant studies, we show that GRP undergoes liquid-liquid phase separation via simple coacervation to form biomolecular condensates in salty environments. Cation-π and π-π interactions mediated by periodically placed arginine and aromatic amino acid residues are the primary driving forces that promote phase separation. Interestingly, GRP condensates exhibit ageing by undergoing liquid-togel transition and exhibit adhesive properties, measured through force spectroscopy. Finally, given the drastic changes in pH taking place during the tick bite, we show that pH significantly influences the GRP hydrophobicity via ionic residues, driving notable variations in the coacervation behavior and in shaping the material properties, including striking amphiphilic properties, of the formed condensates. These findings provide a starting point to gain insights into the adhesion of ticks, develop novel tick control strategies, and towards biomedical applications such as tissue sealants.

Keywords: bioadhesion, biomolecular condensates, intrinsically disordered proteins, liquid-liquid phase separation, ticks

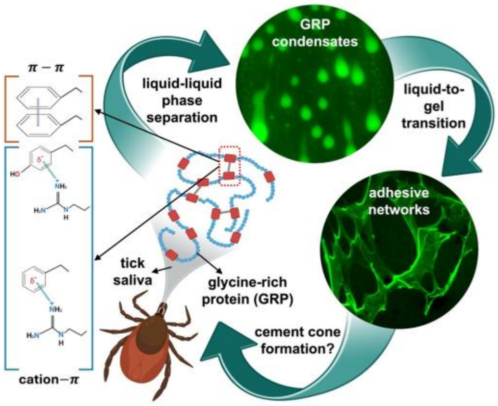

Figure 1. *Schematic overview of GRP phase transitions and underlying driving forces, hinting at their role in tick cement cone formation.*

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Transmission of Mechanical Shear Signals in the Epithelial Layer

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Epithelial tissue is one of the most common tissues in the human body, lining all organ surfaces and internal cavities. These tissues play a central role in maintaining barrier integrity and homeostasis across organs, while also demonstrating plasticity that supports key processes such as embryonic development and wound healing[1]. In the body, epithelial tissues are frequently exposed to mechanical stimuli in various forms and across a wide range of scales—from whole-tissue deformations to local forces at the level of individual cells. While many studies have explored the epithelial mechanical response of either large scale tissues[2], or small scale individual cells[3], investigations at the mesoscale—comprising hundreds to thousands of tightly interacting epithelial cells—remain scarce. To address this, we developed a mesoscopic mechanical probe, based on magnetic tweezers, and examined the epithelial response to controlled mechanical perturbations, and at various stages of maturation. By integrating rheological, dynamical, and morphological characteristics, measured in both short and long time scales, we found that, the more a tissue is jammed and solid-like in appearance the softer it is, and the more it is unjammed and fluid-like in appearance the stiffer it is. Most importantly, the unjammed tissues allow better transmission of mechanical shear signals. Hence, the data suggests a new perspective stating that unlike the dynamic and migrating epithelial state that is more susceptible to external mechanical stimuli, the homeostatic state is more stable. This may serve as a clue to why a small and local irregularity that initiates a tumor growth in homeostatic epithelia do not alert the nearby environment and can stably progress.

Keywords: Jamming transition, Mechanical stimulation, Epithelial layer, Cells rheology, Collective cell mechanics, biophysics .

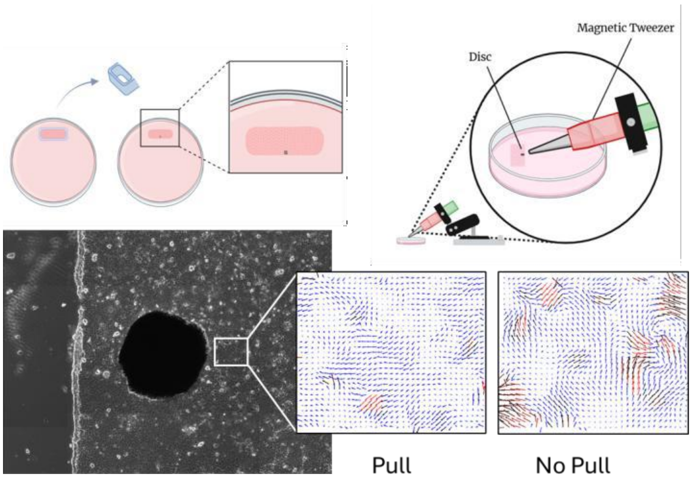

Figure 1. *Experimental setup and comparison of mechanotransducive dynamic arrest with and without mechanical stimuli.*

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Harnessing Shape Fluctuations to Probe the Mechanics of Stress Granules in Live Cells

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Interfacial tension plays a significant role in governing the coalescence dynamics of biomolecular condensates and in determining how condensates interact with and deform lipid membranes and biological filaments. However, approaches for studying them in-situ in living cells under physiologically relevant conditions are not yet well established. Here we present a high-throughput flicker spectroscopy approach to determine the interfacial tension of thousands of condensates inside living cells (Figure 1). Demonstrating this approach on stress granules, we discover that an interfacial tension-only model is inadequate for describing stress granules in live cells. We find that the measured fluctuation spectra require an additional bending rigidity parameter, which has not previously been described for biomolecular condensates. We further observe that stress granules do not have a spherical base-shape but fluctuate around a more irregular geometry. These results demonstrate that stress granules are complex, viscoelastic droplets with a structured interface, rather than simple Newtonian liquids. Moreover, the approach can distinguish between stress granules induced by different chemicals or under different stoichiometries of constituent proteins, based on their characteristic distributions of interfacial tension tension and bending rigidity values. The measured interfacial tensions and bending rigidities span a range of several orders of magnitude. As such, different types of stress granules (and more generally, other biomolecular condensates) can only be differentiated via large-scale surveys.

Keywords: Biomolecular Condensates, Interfacial Tension, Bending Rigidity, Stress Granules

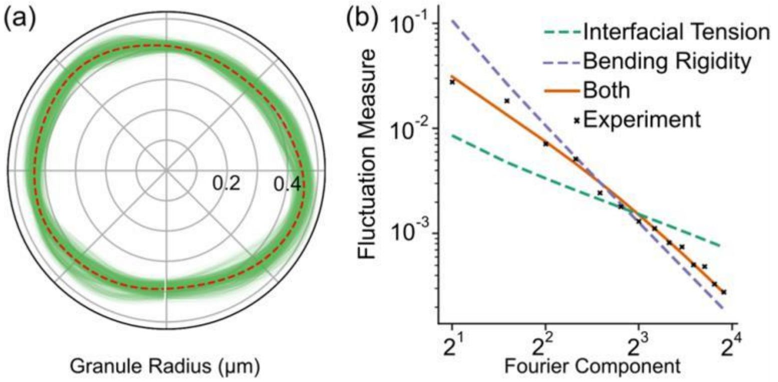

Figure 1. *(a) Typical shape fluctuations of stress granules. (b) The experimental fluctuation spectra can only be explained using a model that has both interfacial tension and bending rigidity.*

Acknowledgements: Funding from EPSRC grant No. EP/V034154/2 and Research Council of Norway grant no. 335901.

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Modifying the mechanical properties of self-assembled filaments by engineering EspA bacterial protein

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Pathogenic bacteria utilize their Type III Secretion System (T3SS) to inject virulence agents/material during infection of epithelium cells in the gastral tract. T3SS is comprised from a long hollow tubular protein filament that forms a syringe like tube, which is anchored into the surface of the bacterium. During the infection process the filament withstands shear stresses induced by the viscous mucosal flow across the gut walls, along normal stresses across it as it stretches between the bacterium and the host cell. Yet very little is known about the physical characteristics of the T3SS that enable its function while maintaining its structural integrity. We investigated the morphological and mechanical properties of EspA filaments and how protein engineering can modify them. Our study included three types of filaments: natural EspA filaments, full-length recombinant EspA filaments, and truncated recombinant EspA filaments lacking a third of the original codon region. The recombinant EspA proteins formed curly, thin filaments with higher longitudinal elasticity (shorter persistence length) compared to the natural, linear filaments. Additionally, the recombinant filaments had a radial elastic modulus about an order of magnitude lower than the natural filaments. The truncated recombinant filaments had a higher radial modulus than the full-length ones, and unlike the purely elastic natural filaments, recombinant filaments were less compliant with the applied force that penetrated them. These differences underscore the potential to modulate EspA filament properties through protein sequence mutations. Our findings suggest EspA as a fundamental element for developing a new biomaterial with a hierarchical structure.

Keywords: Self-assembly, Nanoindentation, Force Spectroscopy, Mechanical properties, AFM.

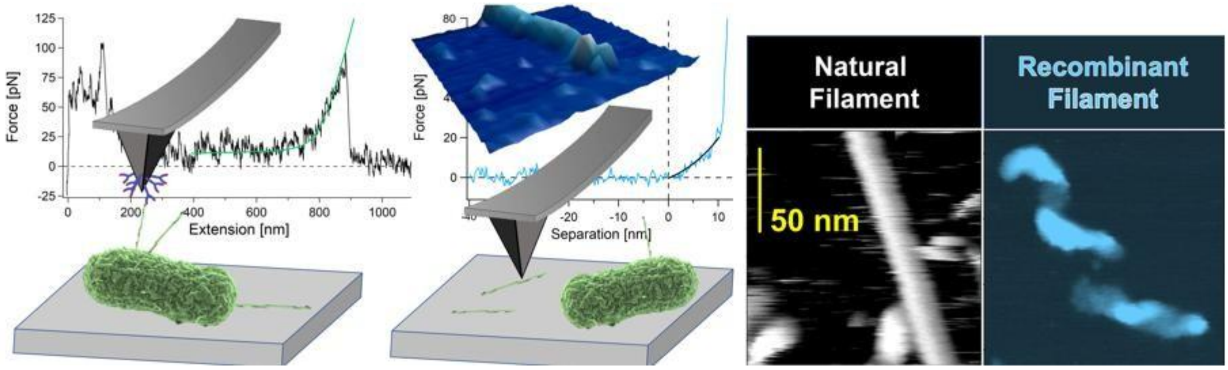

***Figure 1.** Left to right: Schematics of force spectroscopy measurement of pulling a single filament from a bacterium; Schematics of nanoindentation measurement of a single filament; AFM imaging of a single natural filament, and of a recombinant filament.*

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Water in soft confinement of lipidic mesophase

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Water is fundamental to the existence of life. Many biological processes take place in crowded aqueous surroundings, and water in living cells can be considered as confined water. Confining water at nanoscale behaves differently to those in the bulk with respect to the crystallization, nucleation, and molecular dynamics. While in biological systems, the role of confined water is of crucial importance, but still far from fully understood.

Herein, we will discuss the state of water in a soft confining media provided by lipidic mesophase. First, we applied an unfrozen lipid, phytantriol, to form stable lamellar phase at subzero temperatures. Through the combination of differential scanning calorimetry and dielectric spectroscopy techniques, we understood the crystallization and the dynamics of water in such soft confinement. At a lower hydration (< 9.5 wt% of water), the nanoconfined water remains in a liquid state down to -120 °C.[1] On the other hand, the phase structure of lipidic mesophase varies depending on the water content and the temperature of the system. Another interesting question we address is the state of water during phase transitions. We used Fourier transform infrared spectroscopy and dielectric radiation spectroscopy to explore both the static and dynamic states of water network during the phase transition from bicontinuous cubic phases to a reverse hexagonal phase.[2,3]

Keywords: Lipidic mesophase, liquid water, molecular dynamics

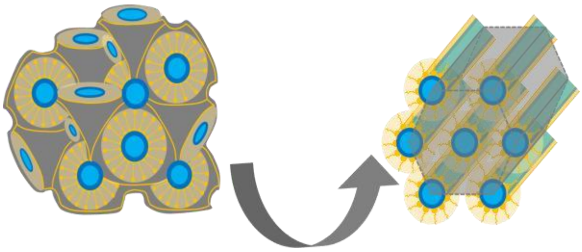

Figure 1. *Phase transition from cubic to reverse hexagonal phase in lipidic mesophase.*

Acknowledgements: Y. Yao thanks the financial support from the Swiss State Secretariat for Education, Research and Innovation (no. MB23.00006).

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Unraveling oleosome interfacial behavior for controlled release of lipophilic cargos

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Encapsulation and controlled release of bioactive agents are essential in the food and pharmaceutical industries. Many bioactive compounds are hydrophobic and must be delivered to a hydrophilic environment within the human body. For this purpose, an ideal carrier should be biocompatible, lipid-based and easily dispersed in an aqueous environment.

Oleosomes, naturally occurring lipid droplets found in plant seeds, are stabilized by oleosin proteins embedded and a phospholipid monolayer. Their inherent emulsifying properties and stability make them valuable in food and pharmaceutical applications. However, a fundamental understanding of oleosomes interaction with lipophilic surfaces and the role of phospholipid and oleosin membrane in oleosome stability remains largely unexplored. In this study, we employ a state-of-the-art microfluidic-based thin film balance to examine oleosome behavior in aqueous thin liquid film (TLF) between two oil droplets. We show that when confined in a TLF, oleosomes remain mobile, with their displacement facilitated by Osmotic pressure gradients and Marangoni stresses (Figure 1a). Cluster formation, facilitated by a balance between hydrodynamic interactions, capillary attraction and electrostatic repulsion results in depleted areas in the TLF that eventually cause film rupture. Importantly, individual oleosomes were found to burst and coalesce with the outer oil phase (Figure 1b). We further covered the surface of the outer oil with lipid-monolayer to mimic outer cell membrane interface and studied oleosome stability at the interface. We systematically investigate the effect of oleosome membrane density on their stability by using a homogenization technique, engineering oleosome membrane with varying surface densities of oleosin and phospholipids. Furthermore, we demonstrate the encapsulation of capsaicin—a lipophilic compound responsible for the heat sensation in chili peppers—within oleosomes. The destabilization of oleosomes, when in close proximity to the hydrophobic oil phase or to a cell-mimicking interface, results in the controlled release of capsaicin, the rate of which can eventually be tuned by oleosin surface density.

Keywords : Oleosomes, lipid droplets, thin film balance, controlled release and interfacial stability.

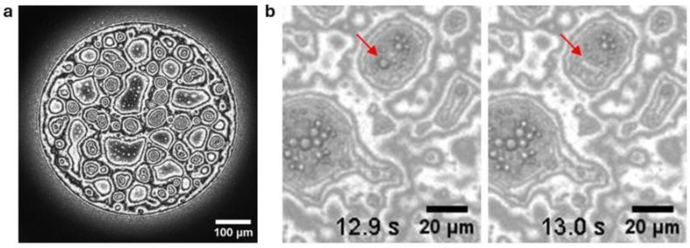

Figure 1: (a) Oleosomes confined in thin film forms clusters. (b) An instance showing trapped oleosomes bursting and coalescence with outer oil phase.

Hidden reticulum of compressed and non-cycling cells reveals epithelial sub-criticality

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As epithelial cells collectively rearrange to heal a wound, or to morph during development, their observable hallmarks are heterogeneities in cell shape and organizational patterns. Structural heterogeneity is conventionally thought to fade as the epithelium matures and gradually transitions to a jammed and solid-like state which is assumed to hold no sign of underlying multicellular processes.[1,2] Our data are contrary to that assumption and expose a heterogeneous and mechanicalstate-dependent reticulum, that evolve with epithelial maturation. Analysis of epithelial monolayers immediately after enzymatic de-adhesion detected polarized mechanical responses and revealed two populations of cells: Large regions of cells under tension, embedded with islands of cells under compression. The islands of compressed cells emerge, and grow in cell numbers, with gradual jamming and with reduced cellular rearrangements. We show how that process is both reversible, by imposing an unjamming and relaxation transition, and inhibitable, by cell cycle arrest treatment. Moreover, studying the spatial patterns of cell cycle state reveals that, within the region of tensed cells, cells preferentially divide. This led to a simple physical model that employs the universal rule that governs a vast host of percolating and complex networks, that is, growth by preferential attachment. The model a priori predicts the dynamic growth pattern of the newly revealed network, or reticulum, and hints that the epithelium self-organizes into a critical state in which perturbations can be transmitted between all length scales. This epithelial criticality provides a new lens to observe and explore fundamental processes in which the homeostatic epithelial tissue is disrupted- from healing of a wound to the initiation of a tumor.

Keywords: Epithelia reticulum, Jamming transition, Compressed cells, Sub-criticality, Hidden morphology.

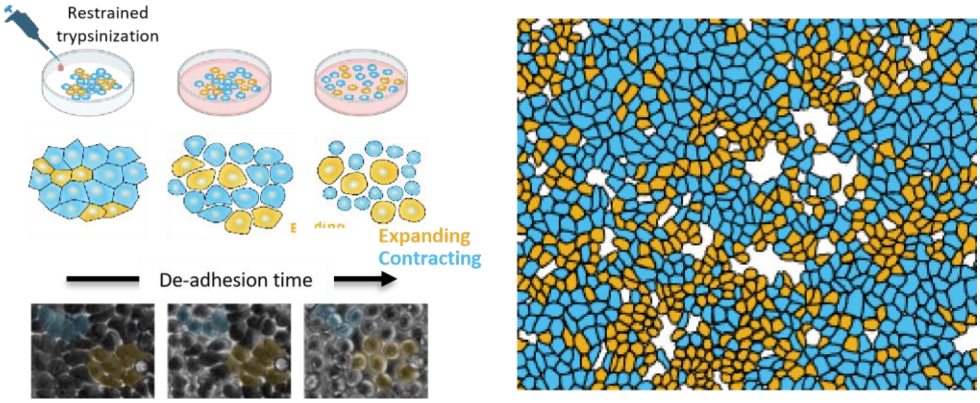

Figure 1. *Enzymatic de-adhesion reveals two mechanically contrasting cell populations: large regions of cells under tension (blue), embedded with islands of cells under compression (yellow).*

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Cytoplasmic Viscosity and Diffusion: Implications for mRNA Translation and Vaccine Delivery

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Producing proteins from mRNA is a central process in cell physiology and mRNA vaccine development, heavily reliant on the diffusion of molecular components such as translation initiation factors, tRNAs, and nucleases. These molecules diffuse in the complex, heterogeneous environment of the human cell cytoplasm, which exhibits gel-like properties at length scales above 100 nm and liquid-like behaviour at shorter scales [1]. We have recently shown that this mesh size can be reduced in response to prolonged starvation [2]. This diffusion hindrance disrupts biochemical pathways, including the complete immobilization of ribosomal large subunits, effectively halting translation initiation. This purely physical phenomenon was observed to serve as a survival mechanism.

In current research, we used fluorescence correlation spectroscopy (FCS) to investigate the impact of lipid-mediated transfection—a common laboratory procedure—on intracellular protein diffusion. We observed fluctuations in protein concentrations lasting tens of seconds, with diffusion rates varying up to threefold at single spots (Fig. 1). Further, we explored the consequences of these intracellular lipid-induced effects on the biophysics of mRNA vaccine candidates. Lipid nanoparticle delivery altered the translation and decay kinetics of external mRNA compared to native cells. In contrast, mRNA delivered via microinjection (a lipid-free method) retained its integrity and activity over twice as long, highlighting the significant impact of delivery methods on mRNA bioavailability.

Our research bridges soft matter physics and biophysics, emphasizing how the material properties of the cytoplasm and delivery formulations influence intracellular diffusion, biochemical pathways, and the efficacy of mRNA-based therapeutics. These insights are critical for optimizing mRNA vaccine design and understanding the biophysical constraints of cellular environments.

Keywords: Diffusion, mRNA, Cytoplasm, Translation, Lipid nanoparticles

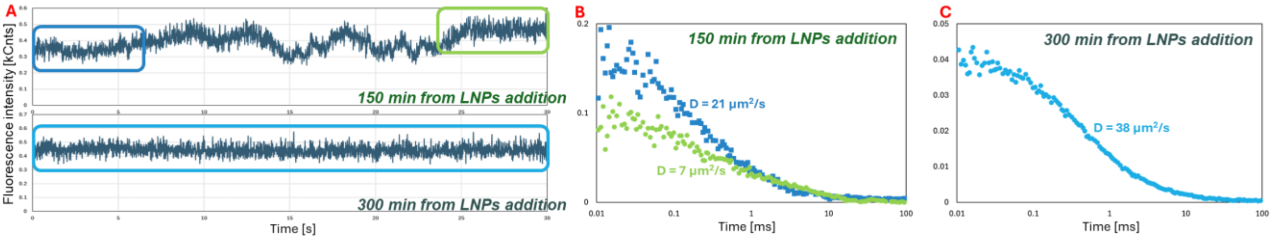

Figure 1. *Intracellular diffusion disturbances upon lipid nanoparticle treatment. (A) significant fluctuations of fluorescence signal from EGFP-loaded cells. (B) Differences in diffusion of EGFP at a single spot within tens of seconds. (C) Cellular recovery after 4 hours post-treatment.*

Acknowledgements: This work was co-financed by the Polish Science Fund, Virtual Research Institute, within the grant WIB-1/2020-O11; WIB_HERO

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DNA packing in viral capsids

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Assembly of viral capsids containing genetic material, is a key process in viral reproduction cycle. The bacteriophages and double stranded DNA viruses assemble their capsids prior to genome packaging and actively push DNA inside by ATP-driven packaging motors. The genome is typically densely packed in the capsid and understanding its spatial configuration presents a challenging problem, which is not completely understood despite its obvious importance.

To elucidate the mechanism of DNA packing, we first explored a simple model of elastic filament confined to a sphere with three competing interactions [1]. The simple phenomenological theory supported by extensive parallel tempering MD simulations of the wormlike chain (WLC) model show that the optimal ground state packing is not an inverse spool configuration as previously assumed; it is a more complex structure where the filament is compartmentalized into multiple domains, resembling nested tori or topological links. While this suggests that DNA will also form multidomain structures in a viral capsid, it is important to realize that DNA cannot be completely described by the linear elastic model. Under sufficient local torsion, the base pairs of the double helix can locally melt creating regions with large flexibility that can easily form kinks. We incorporated this effect into a meltable WLC model and explored nonequilibrium process of pushing such kinkable chains into a capsid by molecular motors [3]. It turns out that the kink formation crucially affects the structure: for sufficiently slow packing process we observe a coexistence of outer spool domain and a twisted nematic core – in a perfect agreement with available cryo-EM experimental observations. Our findings suggest that the nonlinear elasticity of biological molecules plays an important role in their spatial structuring in confined biological systems.

Keywords: DNA packing, nonlinear elasticity, viral assembly

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Physical mechanisms of peptide-mediated inhibition in α-synuclein aggregation

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Protein misfolding and aggregation are associated with the onset of neurodegenerative disorders such as Alzheimer's and Parkinson's disease. To date no cure exists for neurodegenerative diseases and therapeutic interventions give limited symptomatic relief, rather than prevention. An attractive therapeutic strategy is to prevent disease onset is to hinder the formation of toxicity-related accumulations via peptides [1].

Here, we aim to understand the physical mechanisms by which peptides prevent the aggregation of α-synuclein, the protein linked to Parkinson's disease. A better understanding of the physicochemical properties of peptide-modulated assembly mechanisms will aid in the development of the next generation of preventive therapies.

To achieve this, we introduce a novel coarse-grained model for amyloidogenic polypeptides and aggregation inhibitors (Fig. 1) [2] to gain insight into the physical mechanisms of assembly into supramolecular species. We use Brownian dynamics simulations to propagate the dynamics of the system [3].

We find that specific and non-specific interactions modulate the formation of the different aggregates. Additionally, our results show that hydrophobic macromolecules slow down the formation of fibrillar structures. Our results are complemented by biophysical measurements and explain experimental observations.

Keywords: protein aggregation, inhibition, coarse-graining, Brownian dynamics

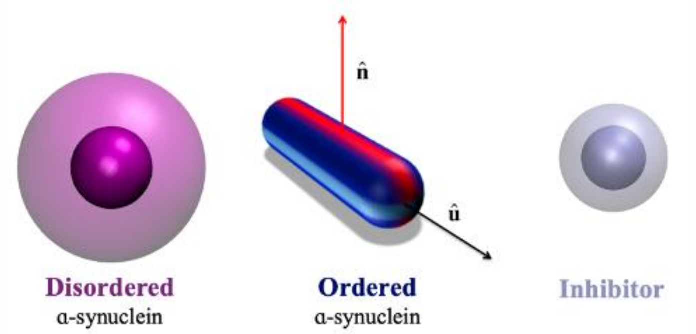

Figure 1. *Coarse-grained models for a-synuclein [3] in the disordered (purple sphere) and ordered states (blue spherocylinder), and generic representation of peptide inhibitors [2] (right).*

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Experimental and Computational Studies of Kinetoplast DNA

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Kinetoplast DNA is a complex structure found in the mitochondria of trypanosome parasites, the cause of Chagas' disease and Leishmaniasis. It consists of thousands of topologically connected "minicircle" that form a two-dimensional network similar to chain mail armour. In the parasite, it serves the biological function of gene editing for mitochondrial RNA. Due to its topologically-complex structure and two-dimensional nature it serves as a unique model system for materials physics.

I will discuss the polymer-like behavior of kinetoplasts from *Crithidia fasciulata* in the context of 2D materials physics, using optical microscopy and atomic force microscopy. Initial investigations showed that kinetoplasts in free solution have a curved equilibrium shape and fluctuate with a very fast timescale that is consistent with the flat phase of 2D polymer physics [1]. More recent experiments based on destructive testing probed the relationship between their underlying network topology and their material properties [2]. I will also discuss recent computational investigations attempting to probe the relationship between network topology and the overall Gaussian curvature that has been observed in confocal microscopy images of kinetoplasts [3]. The results of these simulations suggest a connection between the Calugareanu theorem of DNA topology and the Gauss-Bonnet theorem of surface topology.

Although kinetoplast biophysics is a relatively new field, researchers from a broad range of disciplines typically find the unique structure of kinetoplast DNA and the visually striking behavior it displays to be of great interest.

Keywords: DNA, topology, 2D material, network

Figure 1. *Left: Fluorescence microscopy image of a kinetoplast, scale bar 2 microns. Right. Monte Carlo simulation of a kinetoplast network..*

References

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Friction modifies poroelasticity of a yeast clog

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Soft porous media consisting of assemblies of biological objects are common in many industrial and natural situations. They are often confined, as in the case of yeast clogs trapped in a filtration membrane, or human tumor cells in the case of e.g. bone cancer. Whereas this confinement and the possible friction induced at the boundaries of the porous media are not addressed by the well-known poromechanics theory [1], some recent experimental results tend to prove their importance [2].

For this presentation, we have studied the mechanical properties of a clog of living particles based on observations at the microscale in a model configuration: we used the baker's yeast Saccharomyces cerevisiae, with known mechanical and biological properties, to form clogs that were observed in a quasi-2D microfluidic device with well-controlled dimensions to ensure a high degree of confinement [3]. After the formation of a clog, compression and decompression cycles were applied (see Fig. 1), both in a flow-driven configuration and in an impermeable piston-driven one. The results show that the stress-displacement relationship deviates from the predictions of poromechanics theory and conventional interpretations in the literature, revealing a strong hysteresis. This is the signature of energy loss during the compression-decompression cycle. In addition, complementary experiments show that stress is stored during decompression.

A continuous model is proposed which takes into account the coupling between the fluid flow, the deformation of the clog and the friction against the device's walls. This reveals that the friction magnitude is dictated by a single dimensionless number, that is proportional to the friction coefficient multiplied by the aspect ratio of the device. This model reproduces all the observations remarkably well. Taken together, these results provide a first theoretical framework for the study of bioclogging on small scales and show that friction can have non-trivial effects on the mechanics of confined deformable porous media.

Keywords: frictional poromechanics, bioclogging, microfluidics, yeast

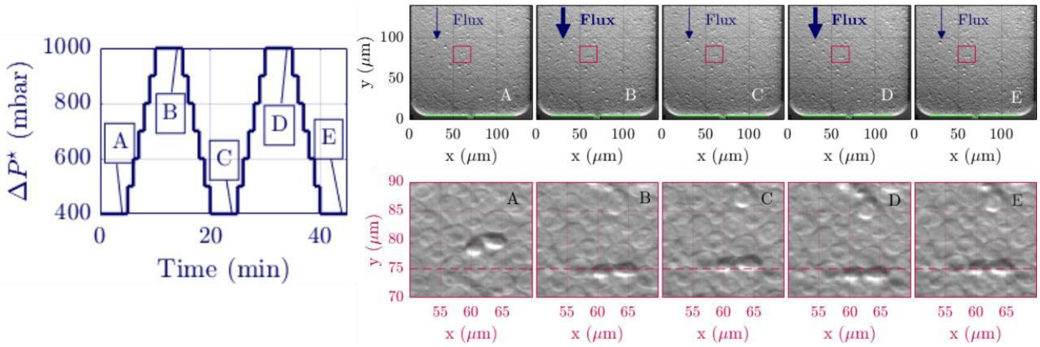

Figure 1. *Left: pressure signal evolution during two cycles. Top-right: micrograph of the clog during pressure evolution at times labelled A-E. Right: zoom on the pink square of the corresponding top-right pictures.*

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Wednesday 1st October 2025

P. Polymers and Networks

(Room 3)

Polyethylene and Polypropylene Take Different Routes to Microplastic Formation

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The formation of micro and nanoplastics by degradation is a topic of considerable concern. It is believed that this form of plastic pollution is highly prevalent and has deleterious consequences for human health and for the environment. Plastics undergo chemical (hydrolysis, UV, enzymatic attack) and mechanical (wind, wave action as well as mechanical attrition) degradation in the environment. We present results on a combination of quiescent degradation (using a modification of an advanced oxidation protocol where potassium persulphate is decomposed to generate free radicals[1]) and shear (by controlling stirring rate using a magnetic stirrer). Here, we focus on the two most widely produced polymers, polyethylene (PE) and isotactic polypropylene (PP).

Under quiescent conditions, both PE and PP become progressively embrittled due to free radical attack. After an induction time, both polymers degrade to form particulate pollutants. We have suggested that the induction time correlates with the essential work of fracture going to zero. In PP, this progresses through free-radical induced chain scission. This results in the formation of microplastic fragments due to embrittlement due to the decrease in the average chain molecular weight. MNP population increases with stirring rate. In contrast, free radical attack results in crosslinking of PE, as evident from melt rheology of the residual PE films. This too leads to embrittlement, but due to chain branching rather than scission. In summary, both PE and PP are embrittled by free radical attack, leading to their fragmentation to yield particulate pollutants. The process of embrittlement for PP arises from chain scission, while this is due to chain branching in PE.

Keywords: microplastic, polyethylene, polypropylene, accelerated weathering

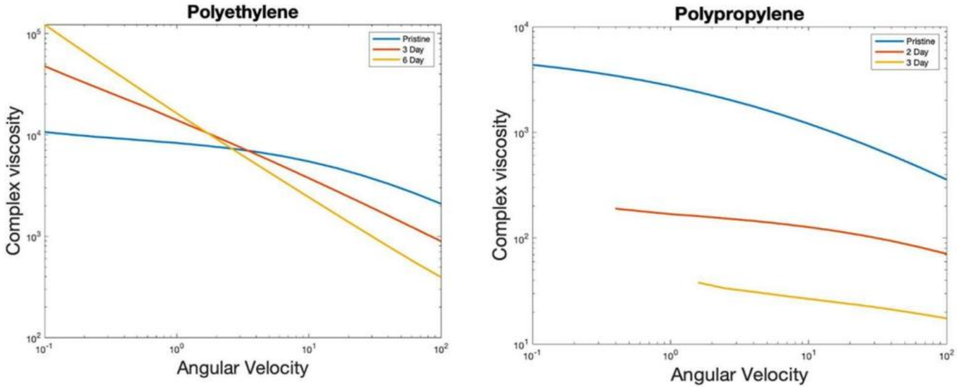

Figure 1. *Dynamic viscosity of melts of (a) polyethylene and (b) isotactic polypropylene as a function of degradation time, during advanced oxidation of films of the polymer samples.*

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Molecular Simulations of Crazes in Glassy Polymers under Cyclic Loading

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Crazing is of considerable technical importance since, unlike cracks, craze fibrils enable load transfer between the craze surfaces and substantially enhance the fracture toughness of glassy polymers. Extensive experimental research for cyclic (especially fatigue) loading exists but their theoretical analysis is difficult without a physically motivated craze model. We study with molecular dynamics simulations the cyclic crazing behavior of glassy polymers [1]. The macroscopic stress response exhibits a hysteresis, which is quasi stationary after the first cycle and largely independent of deformation rate and temperature. It results from a complex interplay between constraints imposed by the entanglement network, pore space and pore space closure. Once the craze fibrils are oriented, stretching of the covalent backbone bonds leads to a rapid stress increase. In the initial stages of unloading, a loss in entanglement contact yields a quick stress relaxation in the backbone. During unloading, the craze fibrils undergo a rigid body (i.e., stress-free) folding motion due to the surrounding pore space, so that the structural behavior of craze fibrils during unloading is most accurately described as string-like. The reloading response depends significantly on the degree of pore space closure and the enforced intermolecular interaction during unloading. It ranges from a linear stress increase to a re-cavitation with a redrawing response. Compared to the bulk stiffness, the craze stiffness is two orders of magnitude lower and as a result, the macroscopic response of coexisting craze and bulk matter is governed by the sole fibrillated craze matter.

Keywords: crazing, glassy polymers, molecular dynamics, cyclic deformation, hysteresis

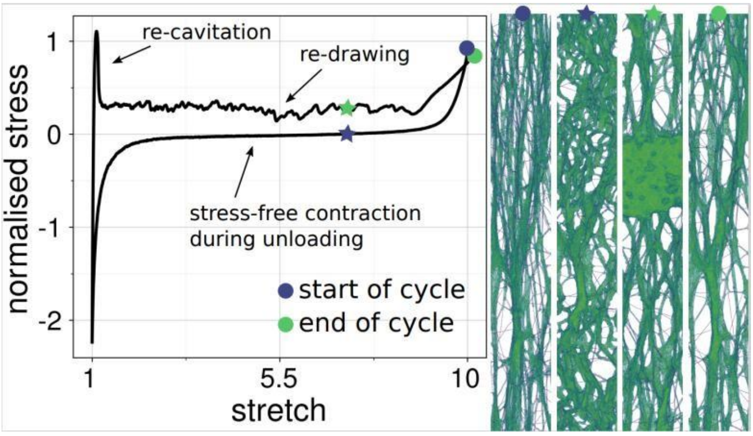

Figure 1. *Stress hysteresis of crazes in glassy polymers subject to cyclic loading. During unloading, the craze fibrils retract via quasi-stress-free motion.*

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Explore hard-to-measure properties of hydrogel with freezing experiments

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Hydrogels are versatile materials with diverse applications. Their high-water content ensures biocompatibility similar to natural soft tissues and allows diffusion of water-soluble molecules, ideal for drug delivery, catalysis, and sensing. Additionally, significant volume changes make hydrogels valuable as bio-inspired actuators in soft robotics and absorbents.

While standard tests exist for many hydrogel properties (e.g. Young's modulus and thermal conductivity), rather surprisingly, it is still very challenging to measure permeability – the key parameter controlling how liquid flows inside hydrogels. In particular, very few experiments have quantified permeability as a function of polymer content. This gap is significant because permeability influences critical processes including swelling, drug release, actuation, and tissue physiology. Furthermore, accurately determining permeability-polymer content relationships is essential to validate theoretical models and optimize hydrogel performance.

Here, we present a novel freezing-based method to directly measure hydrogel permeability. By embedding small hydrogel particles in ice, we exploit cryosuction—a process where ice formation draws water from the hydrogel [1]. When a temperature is applied across a hydrogel embedded in ice, cryosuction sucks water from the warm side of the hydrogel towards the cold side. This causes the hydrogel to move through the ice in the opposite direction. By observing the speed that the hydrogel moves, and relating it to the temperature gradient, we extract the hydrogel's permeability. When we perform the experiment at different temperatures, we can also extract the permeability as a function of the gel's polymer content. I will also show how we can use these experiments to extract a hydrogel's bulk modulus – another crucial mechanical property.

This high-resolution technique requires minimal sample volumes $O(\mu L)$ and offers a robust method for measuring permeability and bulk modulus of hydrogels. These are vital to know for accurate of modelling of hydrogel behaviour, which has long relied on untested theoretical predictions.

Keywords: Hydrogel, Bulk Modulus, Permeability, Cryosuction

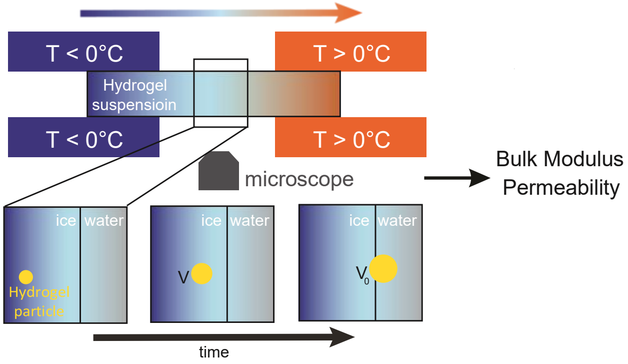

Figure 1. *Illustration of freezing experiment for measuring bulk modulus and permeability of hydrogel. Hydrogel under temperature gradient dT (pressure gradient) move from colder region to warmer region, resulting in change of volume and velocity, which can be used to calculate bulk modulus and permeability.*

References

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Phase separation in elastic polymer networks

Takahiro Yokoyama [1,2], *Yicheng Qiang*[3], *Chengjie Luo*[3], *Oliver Paulin*[3], *David Zwicker*[3], *and Arash Nikoubashman* [1,2]

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Phase separation in polymer networks has received increasing attention due to its important role in influencing the structural and mechanical properties of materials, such as the formation of biomolecular condensates within cells. While previous experimental [1] and theoretical [2] studies suggest that the mechanical properties of the elastic polymer networks regulate phase separation of the network itself and of the embedded (complex) liquid, the fundamental principles governing this interaction remain poorly understood.

To address this knowledge gap, we used molecular dynamics (MD) simulations to explore the phase behavior of polymer networks. We systematically changed the quality of the (implicit) solvent, polymer chain length, and polymer flexibility. Our simulations identified two distinct phase separation scenarios in poor solvent depending on the polymer flexibility: for flexible polymer chains, we found macroscopic phase separation into a polymer-rich and polymer-depleted region, where few chains became very extended to lower the overall polymer-solvent interface (Fig. 1a). In contrast, semi-flexible chains formed networks with finite-sized pores (Fig. 1b), which became smaller with increasing chain stiffness and shorter chain length. Furthermore, the network elasticity increased with decreasing pore size, following a power law in the entropy-dominated regime, consistent with a recently proposed field theory.

Our study highlights the importance of microscopic polymer conformations deriving from, *e.g.*, chain stiffness and chain length, in shaping the size and distribution of droplets within networks.

Keywords: phase separation, elastic polymer network, chain stiffness, semi-flexible chain

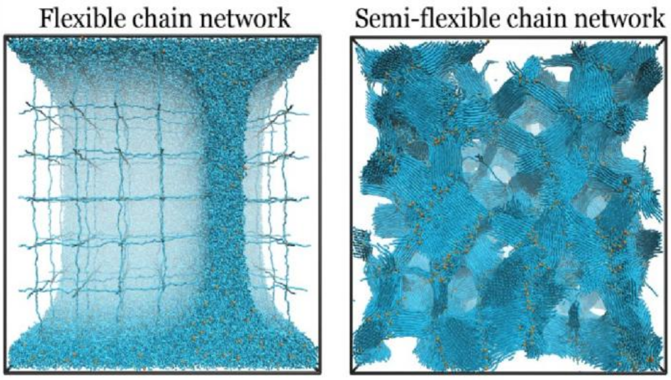

Figure 1. *Phase separation behaviors of (a) flexible and (b) semi-flexible chain networks.*

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Exploring the role of defects in polymer networks formed by star polymers through simulations

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We investigated the role of defects in tetra-PEG (tPEG) polymer networks through coarse-grained molecular simulations. We considered both homoleptic and heteroleptic systems, representing noncovalent bonds between functionalized end groups through an inverted Gaussian potential to control valency. We purposefully introduced connectivity defects in the network by either deactivating some functional groups on the stars or by deviating from the ideal stoichiometry in the heteroleptic mixtures (see Figure 1).
The resulting network structure was quantified using the structure factor, radial distribution functions of attractive beads, and internal loop structures. Polymer mobility was measured through the mean square displacement of individual tPEG molecules post-gelation. We found that connectivity defects change the topology of the network by introducing loops in the system and also enhances the mobility of the star polymers in the network. Higher connectivity defects in the system make the network less viscous and showcases lesser resistance to stress relaxation. Additionally, we varied the bending stiffness of the polymers, observing a significant slowing down with increased stiffness.

Our findings provide new insights into the role of defects in governing the structure, dynamics, and mechanical response of polymer networks.

Keywords: Engineering defects, polymer network, molecular simulations

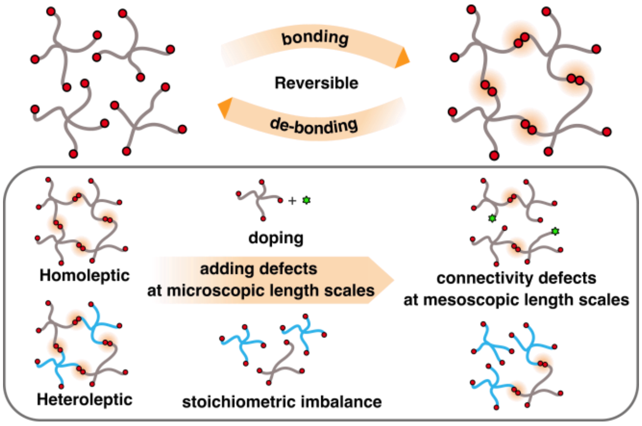

Figure 1. *Protocol for creating the polymer network and engineering defects into the system.*

References

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Understanding the increased failure toughness of double network hydrogels

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Double network hydrogels show remarkable mechanical properties, in that they combine sufficient stiffness to bear load with a high strength and fracture toughness, despite the fact that they contain only a low density of cross-linked polymer molecules in water. This talk will discuss a simple mesoscopic model of a double network material, which is detailed enough to resolve the key microscopic physics of local plastic bond breakage, and yet also simple enough to address macroscopic cracking and its suppression. It will show in particular that load sharing between the two networks results in the stress being delocalised. The mechanism that underlies this is a reduction in the Eshelby stress propagator between sacrificial bonds [1]. This reduction inhibits the tendency for the plastic failure of one sacrificial bond to propagate stress to neighbouring sacrificial bonds and cause a follow-on cascade of breakages. This suppresses the basic mechanism of brittle macroscopic cracking and leads instead to ductile deformation via the formation of many microcracks spread diffusely through the material. In this way, the double network inherits both the stiffness of its stiff-but-brittle sacrificial network and the ductility of its soft-but-ductile matrix network.

Keywords: ductile, brittle, fracture, hydrogels, plasticity

References

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Complex coacervation in complex environments

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The incorporation of complex coacervates composed of highly charged polymers is leading to the development of new soft materials in fields such as energy transition and biomedicine. Charged interactions in biopolymers are also widely used by nature to guide and control delicate biological processes. Yet, the connection between theoretical modeling and experimental material design is still at its infancy in this area due to the richness of interactions in complex coacervation, particularly in out-of-equilibrium conditions often encountered in experiments.

In this talk I will discuss several molecular dynamics simulation works on the behavior of complex coacervates in complex environments, including how the salt resistance and coacervate properties (density, interfaces, chain and glassy dynamics) are affected by the presence of macromolecular crowders or external electric fields. I will also show how this computational information can be leveraged for experimental material design, as shown in a recent simulation-experiment collaboration.

Knots in polymer molecules under Couette & Poiseuille flow

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Knots in polymers and biological macromolecules, such as DNA and proteins, are crucial to their structure and function. However, the effect of external forces on knots existing in polymers is still insufficiently understood. Here, we investigate the impact of shear and Poiseuille flow on knotted flexible polymers using Molecular Dynamics (MD) and Multi-Particle Collision Dynamics (MPCD) simulations [1].

We find that under simple shear (Couette flow), initially loose knots in polymer coils tighten beyond a critical shear rate. Further increase of the shear rate leads to tumbling motions of the chains in flow and fluctuating knot sizes. In contrast, knotted polymer globules subjected to shear unfold into pearl-necklace-like conformations, whereby knots spread across multiple sub-globules and undergo dynamic topological transitions.

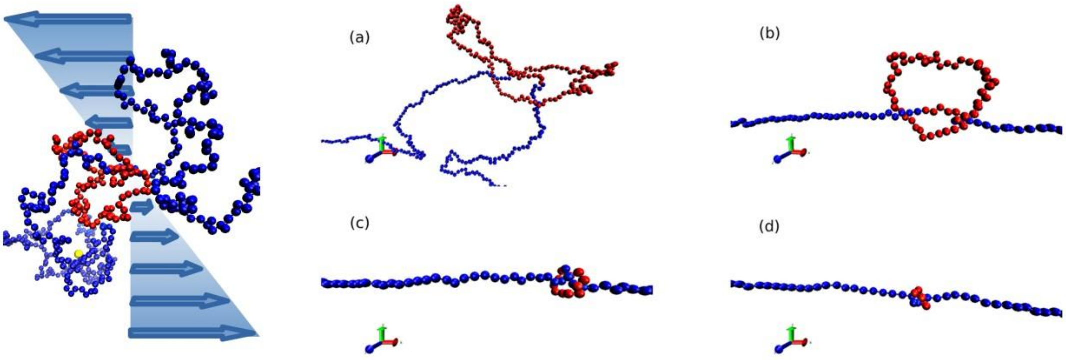

Figure 1. *(left) A polymer chain experiencing Couette flow represented by the blue arrows, with a trefoil knot highlighted in red. (right) A typical time evolution of the knotted region of the polymer chain under Couette flow. The initial trefoil knot is tightened over time while the chain stretches.*

In Poiseuille flow, knots also tighten under increasing flow strength, with fluctuations in knot size emerging at high shear rates. Unexpectedly, the channel width significantly influences the tightening process even at constant mean shear rate.

These findings reveal that both Couette and Poiseuille flow induce major structural and topological transformations in knotted polymers, offering insight into the behavior of knots under hydrodynamic forces in confined and driven environments.

Keywords: Polymer physics, Knot dynamics, Shear, Poiseuille flow, Molecular dynamics, Multiparticle collision dynamics

References

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Non-universal feature of nonlinear rheological behaviour of unentangled polymer melts

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Viscoelastic properties of homogeneous polymeric liquids have been one of the central research subjects in polymer physics. Extensive experiments in the early days established that the properties related to terminal relaxation are determined by just a few molecular parameters irrespective of the chemical structure and concentration of the polymers. In this sense, those properties have been suggesting a universal character in both linear and nonlinear regimes.

Nevertheless, a serious breakdown of the universality was experimentally found in the steadystate elongation viscosity of the simplest model systems such as the melt and semidilute solution of entangled linear polystyrene (PS) with narrow MWD. Extensive studies have examined the molecular origin(s) of the lack of universality from both experimental and theoretical points of view. Some of those studies consider that reducing the friction coefficient ζ of monomeric segments in an oriented/stretched environment is the crucial factor leading to the difference between the solutions and melts of various chemical structures.

The breakdown of universality was also found in the linear viscoelastic regime of the entangled linear chains; the difference in the constraint release (CR) times of PS and polyisoprene (PI) was experimentally pointed out, but its molecular origin remains unclear.

In this talk, we will review the non-universality of polymer dynamics found in linear and nonlinear viscoelastic regimes, introduce our recent studies on these subjects, and further discuss he significant influence that the chemical structure of polymers (and solvents) may exert on polymer rheology.

Keywords: extensional rheology, polystyrene, entangled polymers, polymer melt, semidilute solution, segmental friction coefficient

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Branches, Tie Chains and Entanglements in Bimodal Polyethylene Single Crystals under Uniaxial Tensile Strain

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Using coarse-grained molecular dynamics simulations and a united-monomer model of PE [1], single well-aligned multi-lamella cyrstals were grown [2]. Their lamellar thickness can be controlled by the inclusion of short chain branches. In this presentation we will discuss the uniaxial deformation of these structures to mimick tensile testing. We compare multi-domain structures from continous cooling with the large-scale lamellar structures obtained from a self-seeding protocol [2]. During deformation, the cryatllinity, tie-chain segments, entanglements and folds are monitored and correlated with the stress-strain behaviour and mechnaical properties. At small strains, the single well-aligned PE crystals reveal a larger Young modulus when the deformation direction is perpendicular to the global stem direction. At large strains, the memory of the initial crystal topology plays little role in the mechanical response and is observed to be completely destroyed. Short chain branching appears to suppress disentanglement and shear induced alignment of the chains during deformation. As a result, tie-chains and entanglements persist in branched systems and the peak stress at failure is found to be proportional to the change in number of tie-chains from the beginning of the brittle break to its end. Our findings suggest the remarkable mechanical properties of bimodal branched PE result directly from tie-chains, with entanglements playing a secondary role in the mechanical response.

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Can rheology identify the crosslinking mechanism in polymeric hydrogels?

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Viscoelastic materials may undergo a transition from a viscoelastic liquid (*sol*) to a viscoelastic solid (*gel*). This gelation process is the outcome of a percolative process initiated by the formation of clusters due to the induced interactions between individual molecules. At the transition point, known as the critical gel point (GP) separate clusters percolate to form an "infinite" cluster whose size encompasses the entire system. The ensuing networks can be formed by a variety of chemical reactions or physical processes. The percolative phase transition defined by the GP is a critical phenomenon with universal critical exponents. Winter and Chambon (W-C) [1] argued that at the GP, both *G'* the linear elastic modulus and *G"* the linear viscous modulus obtained by small amplitude oscillatory shear (SAOS) experiments, exhibit the same power law dependence with respect to the angular frequency, *ω*, given by

$$G_C^{'} = \frac{G_C^{''}}{\tan(n\pi/2)} = S\Gamma(1-n)\cos(n\pi/2)\omega^n$$

Here ***n*** is the critical relaxation exponent, ***S*** is the gel network strength, Γ(1-n) is the Euler gamma function, and the subscript *c* denotes the value at the critical point. It was demonstrated that chemical and physical crosslinks are characterized by the same spread in *n* values, and systems with similar physical crosslinking mechanism show a diversity of *n* values. It is evident from the large amount of literature available that by employing linear rheological measurements one can determine P_c, the critical value of the degree of crosslinking at the GP, the associated critical exponents and limited information regarding the structural properties of the crosslinked systems. Details concerning the crosslinking process and the type of junction zones being formed are unattainable from linear rheology.

PVA hydrogels may be readily formed by several methods of chemical and physical crosslinking yielding mechanically stable hydrogels. Covalent chemical crosslinking is achieved by reaction of the hydroxyl groups along the polymer backbone (vulcanization) with one of several appropriate crosslinkers. There are also several methods for physically crosslinking PVA such as complexation with Borax or freeze/thaw cycles. In this work we show that non-linear rheology by means of large amplitude oscillatory shear (LAOS) experiments, supported by Chebyshev coefficients and Lissajous-Bowditch plots, highlighted pronounced differences in nonlinear responses, underscoring the influence of crosslinking mechanisms on material's rheological behavior. The findings establish LAOS as a powerful tool for differentiating polymeric network structures, providing insights beyond conventional linear rheology.

Keywords: gelation, crosslinking mechanisms, hydrogels, critical sol-gel transition, SAOS, LAOS

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The Role of Charge Regulation in Protein Adsorption

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In this presentation we review our recent progress made in understanding the interaction of pHsensitive proteins with a pH-sensitive polyelectrolyte brush. To this end, we employ coarse-grained models of polyelectrolytes and proteins that are simulated with the recently introduced grandreaction Monte Carlo method [1]. This method allows to study chemical equilibria involving weak acid and/or base groups in two-phase systems. We first discuss results that show that the proton concentration inside a polyelectrolyte brush can be markedly different from the bulk concentration, leading to pK$_a$ shifts of several units, in close agreement with experimental results [2]. The system also shows a preferred uptake of divalent ions by the brush, ultimately leading to a hitherto unobserved two-stage swelling of the brush as a function of the pH in the presence of divalent salt. This phenomenon arises as a consequence of charge regulation and ion partitioning [3]. Using small pH-responsive spherical ampholytes as simple toy protein models we show the existence of an optimal uptake value of the pH buffer solution [4]. Furthermore, we show that varying the salt concentration can broaden the uptake window and shift the maximum uptake to higher pH values. The charge regulation capacitance can be employed to tune the selective adsorption capabilities in ampholyte mixtures with similar isoelectric points. Lastly, we discuss patchy protein models that mimic real proteins more closely. We demonstrate that not only charge regulation but also the structure of the charged patches are important factors in driving protein adsorption. Our results give important insights into the tunability of the various forces driving the adsorption and provide guidelines for selective protein purification via electrostatic interactions in brushes or networks [5].

Keywords: protein adsorption, charge regulation, polyelectrolyte brush

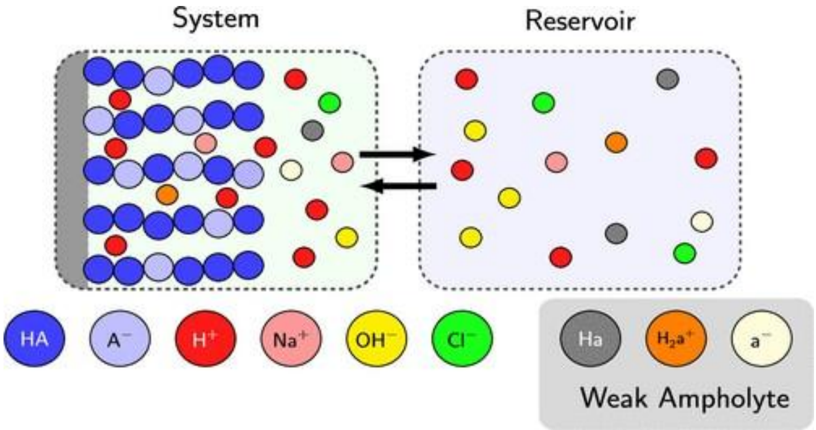

Figure 1. *Schematic representation of the grand-reaction ensemble employed [1].*

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Wednesday 1st October 2025

L. Liquid crystals and anisotropic matter

(Room 4)

Hierarchical Self-assembly of Simple Hard Polyhedra into Complex Mesophases

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Nature offers many intriguing examples of hierarchically self-assembled mesophases, such as lamellar, gyroid, hexagonal, and cholesteric phases. These structures are typically believed to emerge from complex, competing enthalpic interactions, as observed in block copolymers and amphiphilic surfactants. Here, using extensive Monte Carlo simulations, we demonstrate that even simple achiral hard particles with distorted tetrahedral shapes and purely excluded-volume interactions can spontaneously self-assemble into a diverse range of mesophases and liquid crystal phases, including the unexpected emergence of chiral structures.

We attribute the formation of these phases to geometric frustration in the orientational ordering of neighboring particles, induced by their particle shape. The system resolves this frustration by coupling it with an energetically less favorable elastic deformation mode in the orientational ordering, such as twist or splay. We show that simple shape descriptors, such as anisotropy or biaxiality, predict the self-assembly behavior: rod-like particles stabilize cholesteric and twisted lamellar phases, plate-like particles form biaxial and splay nematic phases with randomly distributed splay domains as well as hexagonal cylindrical phases, while moderately anisotropic particles favor gyroid phases. This framework provides valuable insights for designing mesophases in supramolecular chemistry, liquid crystals, colloid science, and nanoparticle assembly.

Keywords: liquid crystals, self-assembly, mesophases

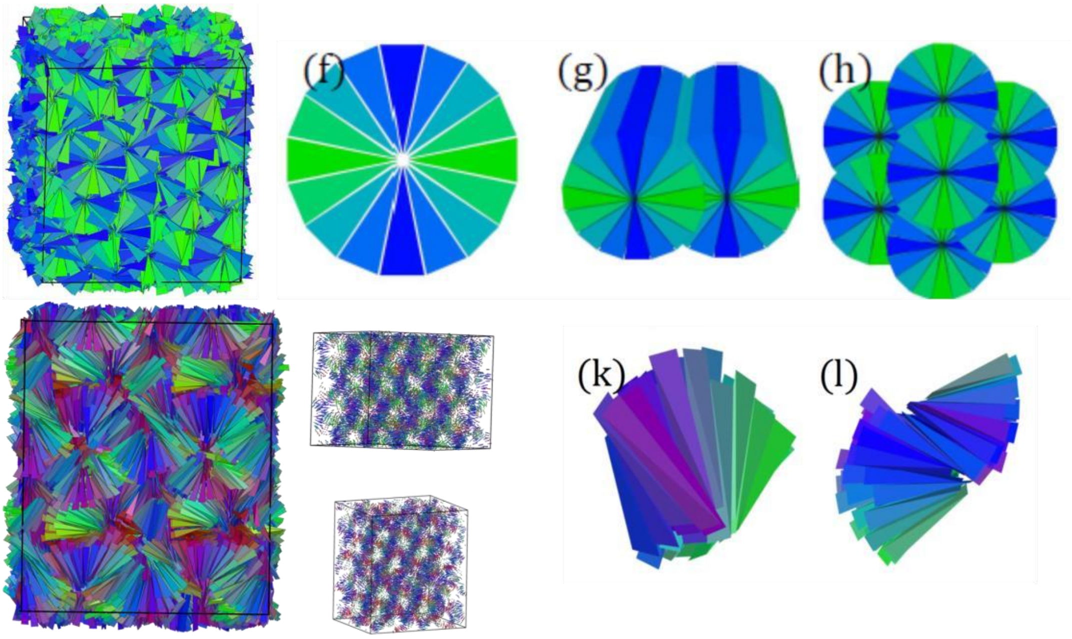

Figure 1. *Hexagonal columnar phase with a schematic of particles forming closed circular assemblies, which stack vertically to create multiple stacks that organize into a hexagonal lattice of interpenetrating columns (top). Single gyroid phase composed of saddle-splay assemblies that anti-align (bottom).*

The assembly of chiral ureido-pyrimidinone-based supramolecular polymers

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Liquid-liquid and liquid-liquid crystalline phase separation (LLPS and LLCPS) are fundamental processes vital for many biological and physical phenomena. Under different stimuli, such as pH changes, salt concentration, and the introduction of non-adsorbing compartments, a mixture of nonisotropic entities may spontaneously phase separate and assemble into higher hierarchies of order by forming nematic islands known as tactoids surrounded by an isotropic phase. Tactoids can be classified as homogeneous, bipolar, and chiral [1]. These entropy-driven assemblies are well established theoretically by Onsager and others [2,3] and thoroughly investigated experimentally in polymer and colloid sciences [4,5]. Recently, a pioneering work presented these fundamental principles in supramolecular polymeric systems for the first time [6]. Herein, the assembly of chiral ureido-pyrimidinone (UPy) motifs was investigated in the presence of different depletion agents and under different environmental conditions, aiming to unravel the sufficient and necessary conditions for the formation of different types of tactoids. Controlling the shape, aspect ratio, and chirality of such systems is of great importance for both fundamental research and applications. The insights gained from the observations will be discussed in the context of the molecular origins of the effect and the mesoscopic level.

Keywords: LLPS, tactoids, supramolecular polymers.

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Origin of chirality in the cholesteric phase of virus suspensions

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Chirality is ubiquitous in Nature, and it exists across all observable length scales, starting from the molecular level where broken enantiomeric symmetry in L-amino acids and D-sugars can generate helical secondary structure in proteins and DNA, and through to the supramolecular level where it creates macroscopic chiral architectures including most of living matter. These chiral morphologies are significant not only in biological systems, but have important implications for materials and nanoscience, including photonics, enantiomeric separation, optoelectronics and sensors.

The key question of how chirality propagates from nanoscale building blocks to high-order helical assemblies remains a major open issue, despite many investigations over the past decades [1,2]. Working with a model system of chiral rod-like particles, the filamentous fd viruses widely used from biology to materials science, we demonstrate that their self-assembly into chiral liquid crystal phases results from the interplay between three main mechanisms of chirality amplification that will be presented and discussed quantitatively [3].

Our work highlights the ways in which supramolecular helicity may arise from subtle chiral contributions of opposite handedness that act either cooperatively or competitively, thus accounting for the multiplicity of chiral behaviors observed for nearly identical molecular systems [3].

Keywords: Colloidal Liquid Crystals, fd Virus, Chirality, Helicity.

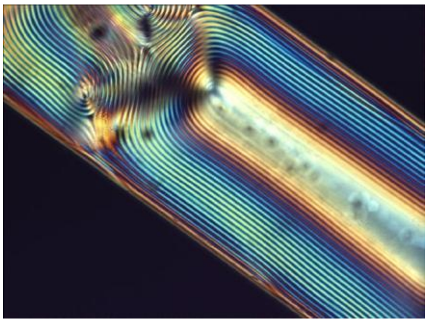

Figure 1. *Optical microscopy image observed between crossed polarizers of the chiral self-assembly into cholesteric liquid crystalline phase formed by an aqueous suspension of filamentous viruses showing the typical fingerprint texture. Scale bar is provided by the width of the experimental cell, which is 1mm.*

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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.

Keywords: Chirality, Liquid Crystals, Polydispersity, Colloids, Molecular Dynamics

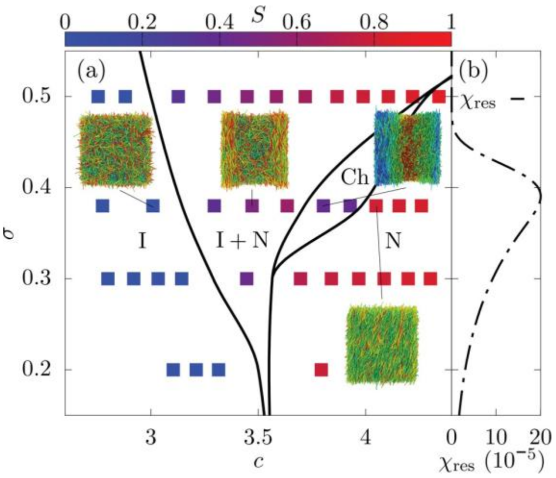

Figure 1. *(a) Phase-diagram of soft repulsive near-rigid rods in the polydispersity-concentration ($\sigma - c$) plane. Points colored by global nematic order S. A spontaneously twisted cholesteric phase emerges at intermediate σ. (b) Residual chirality χ_{res}, predicted from a theoretical model, peaks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

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Entropy stabilized form chirality in curved rod nematics: structure and symmetries

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The nature of the nanoscale form chirality exhibited by so-called dimer liquid crystals—mesogenic cores connected by a flexible spacer chain—is a contentious subject [1-3]. In 2011 it was claimed [4] that the "N_X phase" is the long-lost the twist-bend nematic proposed by Robert Meyer in 1972 [5]. However, coarse grain modelling of dimers using Monte Carlo simulations of achiral curve-shaped rods exhibit polymorphism revealing both smectic and polar nematic phases. A locally-chiral, nanoscale modulated structure forms in the Nx phase characterized by a unique, polar, C_2-symmetry axis that tightly spirals generating a mirror-symmetry-breaking organization of the achiral rods—form chirality [6].

A comprehensive characterization of the polarity and its symmetries in the Nx phase confirms that the nanoscale modulation is distinct from the elastic deformations of a uniaxial nematic director in the twist-bend nematic phase proposed by Meyer. Instead, analogous to the isotropic-to-nematic transition, entropy stabilizes the roto-translating polar director in the polar-twisted nematic phase (N_{PT}), a new nematic polymorph advanced by Vanakaras and Photinos [7,8]. The origins of the nanoscale modulation in the lower temperature, N_{PT} (= N_X) phase found in dimer liquid crystals is fundamentally different from the macroscale modulation in the twist-bend nematic.

Keywords: form chirality, dimer liquid crystal, Monte Carlo simulations

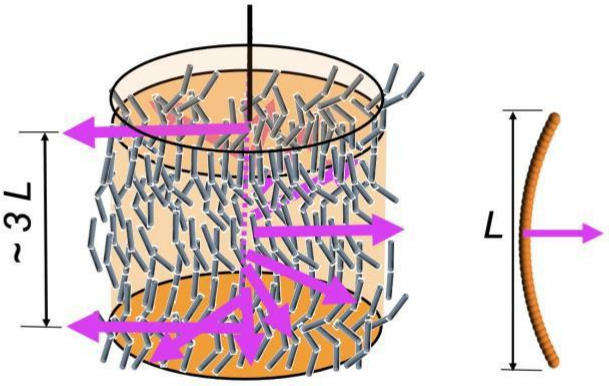

Figure 1. *The polar twisted nematic polymorph with a nanoscale, helicoidal structure.*

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Polymer-stabilized topological solitons formed by low-power light beam in a dye-doped chiral nematic liquid crystal

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In this study we propose a new method for low-power optical generation of localized orientation structures in chiral nematic liquid crystals (CNLCs), including cholesteric spherulites. Cholesteric spherulites are classified as topological solitons, which are of interest as tunable optical elements or components of more complex optical and photonic systems, for example, microlens arrays [1] or two-dimensional diffraction gratings [2].

Well-known studies [3,4] have demonstrated optical generation of topological solitons at a sufficiently high power of the recording light beam of 40 - 110 mW per localized structure. An opto-molecular approach [5], based on the use of a photoactive CNLC with a light-controllable cholesteric helix, has demonstrated the formation of similar topological solitons at a recording beam power of tens of nanowatts. However, this approach required the use of a specific chiral molecular additive and permanent illumination of the LC sample to maintain the existence of the structures.

In our work, we demonstrate a new simple approach for addressable generation of various localized chiral structures, including cholesteric spherulites, using the Gaussian beam with the power of only a few milliwatts. We investigate the generation of localized orientation structures at various parameters of the light beam and frustrated dye-doped CNLC films, as well as the evolution of these chiral structures under an applied electric field. Furthermore, we develop the composition of the polymerizable CNLC matrix. Polymerized pairs of topological defects are shown for the first time, forming in an applied electric field. We emphasize that all metastable topological solitons and nonequilibrium defect structures can be polymerized at any time moment without distorting the director field.

Keywords: chiral nematics, topological solitons, azobenzene dye, polymerizable CNLC matrix

Acknowledgements: This work is supported by the Higher Education and Science Committee of the Republic of Armenia, grant 24AA-1C060.

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Field-Controlled Self-Assembly and Reconfiguration in Multiferroic Liquid Crystalline Colloids

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Recent discoveries of ferromagnetic and ferroelectric liquid crystals have paved the way for designing advanced electro- and magnetoresponsive optical materials [1-3]. We recently demonstrated multiferroic behaviour in colloidal suspensions of scandium-doped barium hexaferrite nanoplatelets within a ferroelectric nematic liquid crystal [4]. A striking consequence of the interplay between ferroelectricity, the vectorial nature of the nematic director, and fluidity is the self-assembly of magnetic nanoplatelets into magnetically switchable network-like microstructures. Switching occurs through soliton-like excitations, where magnetisation flips between poles.

Using optical microscopy in a magnetic field, we characterise the switching dynamics of nanoplatelets in both weak and strong field regimes, as well as under electric field influence. Additionally, we investigate the quenching effect of a magnetic field on the magnetoelectric effect, where an oscillating magnetic field induces an electric response in the multiferroic material.

Keywords: colloids, liquid crystals, ferrofluids, multiferroic

Acknowledgements: The authors kindly acknowledge Dr. M. Klasen-Memmer and Dr. R. Tuffin from Merck Electronics KGaA for providing LC materials and Deutsche Forschungsgemeinschaft for the financial support (Project: NH1668/1-3, ER 467/8-3)

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Shaping nematic order in bacterial films with single-cell resolution patterning

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When growing on a surface, *B. subtilis* bacteria proliferate as cell chains[1] (elongating filaments of constant width) which can locally align with each other upon contact. At high cell density, such microbial population can self-organise in liquid-crystalline domains of aligned cell filaments delimited by topological defects (***Figure 1***). Powered by cell growth, chaotic flows of cells emerge forming vortices reminiscent of liquid turbulence. This dynamical anisotropic matter can be described as an active nematic phase[2].

Here we investigate the dynamics emerging within such 2D bacterial colonies by harnessing the precision of capillary assembly methods[3]. By patterning *B. subtilis* spores with controlled initial spatial configuration at single-cell resolution - namely their positions and orientations, we aim to shape the dynamics and final morphologies of monolayer biofilms. When seeding spores such that the filament out-growth is parallel, we can obtain high nematic order across millimetre scale. Upon growth-induced compression, we observe the onset of active turbulence as the parallel filaments buckle simultaneously. This results in a large-scale alignment of +1/2 topological defects along the axis perpendicular to the initial filament orientation. Such grown thin biofilm exhibits anisotropic optical properties of light polarisation and structural colours.

Controlling the anisotropic nature of the grown biofilm represents a potential opportunity to exploit anisotropic mechanical, chemical, electrical, or optical material properties for useful applications. Achieving predictable microstructural control in nematic biofilms remains highly challenging and could open new doors for the development of biomaterials with high-resolution anisotropy and responsive functions. In addition, improving further our capacity to manipulate the physical arrangement of cells to investigate the effect of different imposed structures can help decipher the implications of spatial structure in microbial communities.

Keywords: Biophysics, Active nematics, Biofilm, Cell patterning, Active matter, Anisotropic matter

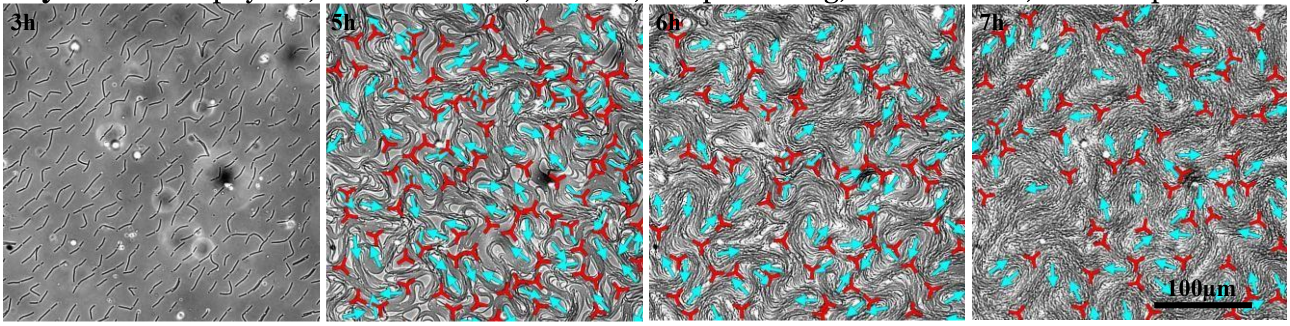

Figure 1. *Active nematic phase emerging from a patterned array of B. subtilis spores growing as a 2D biofilm between PDMS and agarose. The initial pattern is 20um-spaced with parallel orientations. Microscopy images at 3h, 5h, 6h and 7h with +1/2 topological defects as cyan arrow and -1/2 as red trefoil symbols.*

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Flexible, Photonic Films of Surfactant-Functionalized Cellulose Nanocrystals for Pressure and Humidity Sensing

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Most paints rely on pigments that absorb light and gradually fade. A more durable alternative exists in nature, where structural coloration results from light interacting with submicron structures. Cellulose nanocrystals (CNCs), derived from plants, replicate these natural structures by selfassembling into a cholesteric liquid crystal, producing structural coloration upon full evaporation. While CNCs in aqueous solutions have been extensively studied, their transfer to apolar solvents— commonly used in paints—remains less explored. This study uses a common surfactant in agricultural and industrial products to suspend CNCs in toluene. Surprisingly, a stable liquid crystal phase develops within hours, even at concentrations up to 50 wt.%. Evaporating the apolar CNC suspensions results in photonic films with peak wavelengths ranging from 660 to 920 nm. The films are flexible and exhibit varying mechanical properties depending on surfactant content, enabling an optical response to applied force. The films also function as humidity sensors, swelling with increasing relative humidity and causing a redshift in the reflected wavelength. By adding a single surfactant, CNCs become compatible with existing industrial coating production methods while enhancing the strength and responsiveness of structurally colored films to external stimuli.

Keywords: cellulose nanocrystals, cholesteric, liquid crystals, structural color, sensors

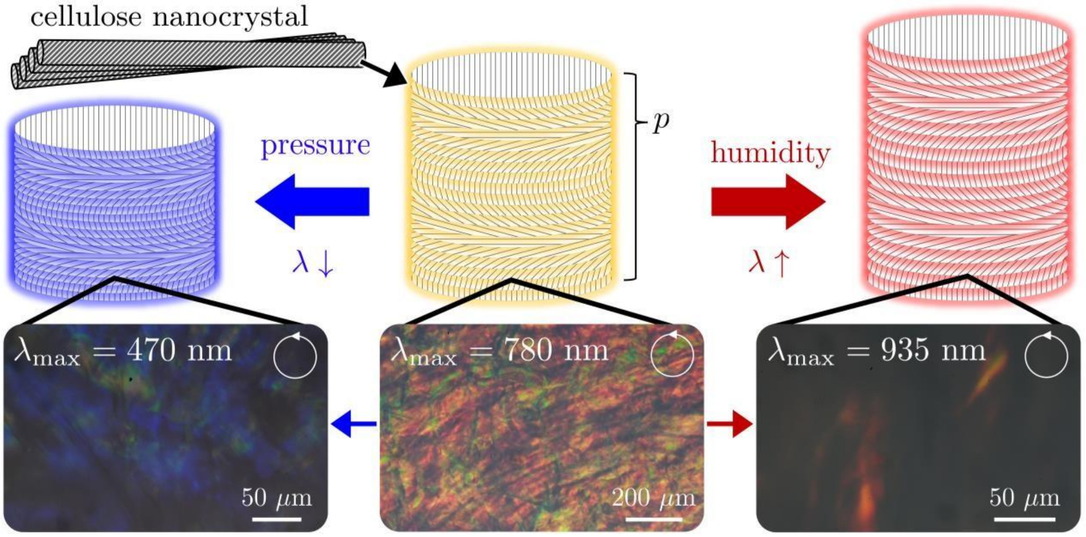

Figure 1. *(top) Schematic illustrating the self-assembly of surfactant-functionalized CNCs into cholesteric films. Cellulose nanocrystals are functionalized with a commercial surfactant STEPFAC 8170-U, allowing for stable dispersions in toluene. When the toluene is slowly evaporated, the CNCs self-assemble into a chiral, cholesteric liquid crystal (yellow). The periodic spacing in the helical ordering is characterized by the pitch p. With applied force (left) or higher relative humidity (right), the pitch can be decreased or increased, respectively, giving rise to a corresponding blue- or redshift in the reflected light wavelength. (bottom) Micrographs of CNC films formed after the evaporation of toluene. The color of a reference film (center), measured via the peak wavelength from UV–vis spectroscopy, can be blueshifted with applied force, F, (left) or redshifted with increased RH (right).*

Liquid Crystal Elastomer Kirigami

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Liquid crystal elastomers (LCEs) are soft responsive materials where orientable liquid crystal units (mesogens) are components of a polymer structure. They present exciting opportunities for soft robotics and environmentally-adaptive systems owing to their heat-responsive deformation capabilities: more than 25% uniaxial contraction when heated uniformly from 25C to 80C. The programmability of LCEs is however challenging, as their material properties and heat-induced deformation are selected during the chemical synthesis that sets the molecular alignment of the mesogens. In effect, LCE structures are typically programmed by macroscopically patterning the mesogen alignment.

Here we take a different avenue, combining macroscopic topology alterations, namely (kirigami) cuts and uniaxially-aligned LCEs to obtain multiscale, responsive metamaterials: LCE kirigami. We investigate LCE kirigami where cuts are oriented orthogonal to the alignment of the LCE sheets. We characterize experimentally the mechanics of tethered LCE kirigami at different temperatures and show that the stress-strain measurements are identical to a canonical tensile test of uniaxial extension of an LCE kirigami. This experimental validation allows us to model and quantify the response of LCE kirigami at different temperatures with conventional mechanical FEM simulations.

We use cut patterns to program the elastic properties of LCEs, while leveraging their heat-response. Further we design structures that deploy under temperature control and reshape in response to temperature patterns. Next, we investigate the recoil dynamics of LCE kirigami and show that non-trivial behaviors result from the interplay between the microscopic structure of the LCEs and the redirection of the stress by macroscopic cuts.

Altogether, we demonstrate that LCE kirigami are multiscale metamaterials that are beyond the sum of their constituents. Macroscopic cuts deform with the isotropic-nematic transition of LCEs, but also redirect stress from along to perpendicular to the LCE director. Our approach highlights the potent role of kirigami cuts when combined with anisotropic materials, setting an uncharted route for soft robotics.

Keywords: liquid crystal elastomers, kirigami cuts, tunable mechanics

Ferromagnetism and Ferroelectricity in Nematic Colloidal Systems

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Recent progress in liquid crystalline colloids has led to the emergence of ferroic fluids that combine magnetic and electric order. Suspensions of barium hexaferrite (BaHF) nanoplatelets in nematic liquid crystals (LCs) exhibit spontaneous magnetisation while retaining fluidity, forming so-called *liquid magnets* or ferromagnetic nematics with unique magnetooptical properties. These materials open new avenues for tunable photonic elements and soft magnetooptic technologies.

A particularly exciting direction involves ferroelectric nematic (N_F) phases, which exhibit genuine ferroelectric order in a 3D fluid. Embedding BaHF nanoplatelets into N_F matrices yields multiferroic hybrids where both magnetisation and electric polarisation can be externally controlled. Magnetisation is stabilised through coupling between the nanoplatelets and the nematic director, forming topologically rich defect networks that guide self-assembly. Magnetic fields not only reorient magnetisation but also modulate polarisation via magnetoelectric coupling, enabling tunable optical non-linearities.

We investigate this coupling and associated optical responses using Second Harmonic Generation microscopy and interferometry. Our study spans dynamic magnetooptical behaviour in ferroelectric and multiferroic suspensions, as well as in ferromagnetic nematic droplets. We further analyse how nanoparticle self-assembly influences defect topology under magnetic fields.

These highly responsive hybrid materials show strong potential for next-generation magnetooptical and magnetoelectrical devices, targeted drug delivery, and in vivo biosensing, offering adaptive functionality through the interplay of magnetism, ferroelectricity, and liquid crystalline order.

Keywords: colloids, liquid crystals, multiferroics

Acknowledgements: The authors kindly acknowledge Dr. M. Klasen-Memmer and Dr. R. Tuffin from Merck Electronics KGaA for providing LC materials and Deutsche Forschungsgemeinschaft for the financial support (Project: NA1668/1-3, ER 467/8-3)

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Magnetic control of driven colloids dispersed in liquid crystals

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Liquid crystals (LCs) are complex fluids that feature long-range orientational order, and studying the propulsion of colloidal entities within them is of interest for their capacity to respond to external stimuli. When colloids are dispersed and driven in LCs, new propulsion phenomena emerge due to the inherent anisotropy of the liquid phase[1]. Furthermore, orientational waves (waves formed by changes in the orientation of molecules within the material) can be generated and propelled through the complex liquid[2,3]. Particularly, studies have shown the possibility of generating solitonic waves that exhibit behaviour close to that of colloidal inclusiong. While the motion of solitonic waves and solid particles within liquid crystals has been explored, there is a lack of in-situ control of their directionality using simple experimental strategies while performing observations.

In this work, we show simple arrangements based on the application of fixed external magnetic fields to control solid polystyrene (PS) particles and two types of solitary waves, both in confined and unconfined LCs. We demonstrate that degeneration in motion directionality can be broken by applying an in-plane fixed magnetic field while running experiments, showing that, for the case of some solitons, the magnetic field has a direct effect on their shape and velocity. In addition to this, we show how to attain dense regions of PS particles in the form of rotating mills, by generating topological defects on the surrounding LC using toroidal magnetic fields, enabling collective behaviour studies. Moreover, some of these colloidal entities are introduced and steered inside microfluidic channels. It is in these systems where we observe a dependency of propulsion velocity on the channel width, a clear phenomenon related to lateral confinement imposed by walls. Consequently, this work gives an approach to the field of colloidal control in complex fluids by magnetic fields.

Keywords: LCEEP, Solitons, Colloidal Particles, Magnetic Field.

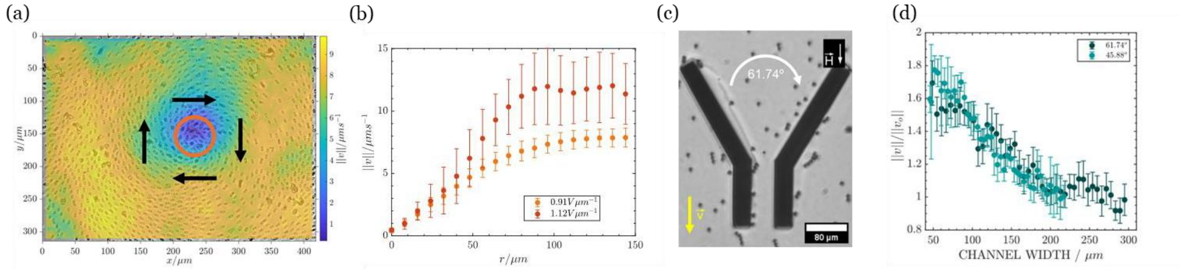

Figure 1. *(a) Rotating mill conformed of polystyrene particles around a +1 defect inside a nematic LC cell. The background color refers to the mean speed in the field of view. (b) Speed variation of the PS particles as a function of mill radius for different propelling electric field amplitudes. (c, d) Normalized velocity variation of solitonic waves passing through microfluidic channels with different aperture angles.*

Acknowledgements: All authors acknowledge funding from project PID2022-137713NB-C21. The presenting author also acknowledges funding from MICIU through the FPU22/01916 program.

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Thursday 2nd October 2025

C. Colloidal matter

(Room 1)

Gauge invariance of statistical mechanics

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A specific shifting operation on classical phase space was recently shown to constitute a gauge transformation for statistical mechanical microstates [1]; popular accounts are given in Refs. [2,3] and a pedagogical introduction is presented in Ref. [4]. The infinitesimal generators of the continuous gauge group form a noncommutative Lie algebra, which induces exact sum rules that relate different microscopically resolved correlation functions to each other. Using gauge invariance in simulations offers possibilities for construction of smart sampling algorithms. The gauge structure points towards a deeper basis of statistical mechanics than previously known, and it offers avenues for systematic construction of exact identities and for making fundamental progress in the dynamical description of colloidal matter in nonequilibrium [5].

Keywords: gauge invariance, Noether's theorem, sum rules, force correlations, hyperforce balance, nonequilibrium

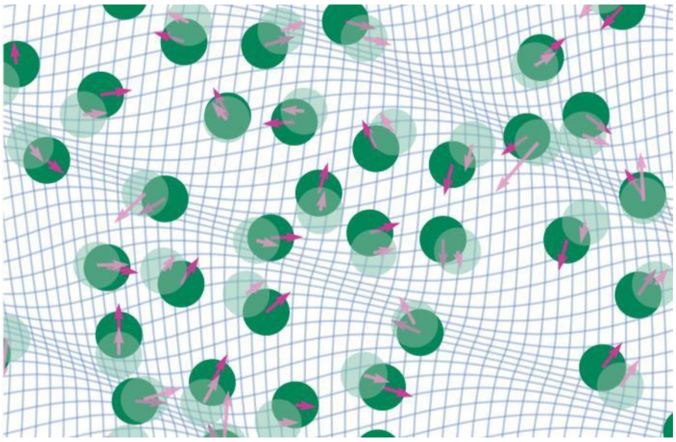

Figure 1. *Statistical mechanical averages are invariant under a specific shifting transformation of positions and momenta of a many-body system. The shifting constitutes a gauge transformation that can be exploited in equilibrium and in nonequilibrium.*

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Star-like thermoresponsive microgels: a new class of soft colloids

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Microgels are soft colloidal particles with micro- to nanoscale dimensions, consisting of a crosslinked polymer network with the ability to respond to various external stimuli, such as light, pH, ionic strength, and temperature. Among the most widely investigated microgels are those based on poly(N-isopropylacrylamide) (PNIPAM), a thermoresponsive polymer that exhibits a volume phase transition (VPT) in response to temperature changes. PNIPAM microgels are typically synthesized via free radical polymerization in the presence of a crosslinking agent, most commonly N,N'-methylenebis(acrylamide) (BIS). Due to the differing reactivities of NIPAM monomers and BIS crosslinkers, the resulting microgels adopt a core-shell morphology, well described by the fuzzy sphere model.

Star polymers, consisting of multiple arms radiating from a central small core, are instead the prototypes of ultrasoft colloids, with an interesting logarithmic dependence of the interaction potential. However, the chemical synthesis of multi-arm stars is quite involved, requiring deep expertise. Furthermore, the polymers used to produce stars are usually not thermoresponsive.

In this contribution I will present recent experimental and simulation results on PNIPAM microgels where the cross linker is ethylenglykol dimethacrylate (EGDMA), building on the pioneering work of Hellweg group back in 2002 [1]. Thanks to the much faster reactivity of EGDMA with respect to BIS, these microgels adopt a peculiar star-like structure at low cross linker concentration, confirmed by the agreement of the measured Small Angle X-ray Scattering form factors with those of star polymers and with monomer-resolved computer simulations of a microgel model, building on our previous work[2]. With increasing concentration of EDGMA, the microgels display an increasing, crosslinkers-rich core, also compatible with simulations based on a monomer-resolved microgel model, and with a complex core-fuzzy shell structure. For all studied EDGMA concentrations, these microgels undergo a very sharp Volume Phase Transition and manifest a high deswelling ability, in contrast with standard PNIPAM-BIS microgels.

Bridging the properties of thermoresponsive microgels and star polymers, these results [3] provide evidence of a new class of soft colloids, which paves the way to the discovery of new fundamental behavior and a high potential for applications.

Keywords: microgels, star polymers, monomer-resolved simulations, soft colloids

Acknowledgements: We acknowledge financial support by Progetto Co-MGELS funded by the European Union - NextGeneration EU under the National Recovery and Resilience Plan (PNRR) Mission 4 “Istruzione e Ricerca” - Component C2 - Investment 1.1 - "Fondo PRIN", Project code PRIN2022PAYLXW.

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Softness dictates the rheology of small colloids

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We carefully study the effect of softness in suspensions of small Poly(N-isopropylacrylamide) (pNIPAM) microgels. The PNIPAM particles have a hydrodynamic radius of 100 nm (in the swollen state). Small and ultra-low crosslinked (ULC) microgels studied here remain fluids well above overcrowding environments. We utilize shear rheology to carefully study the evolution of plateau modulus, yield stress, and yield strain with generalized volume fraction (ζ), Figure 1.

The ULC microgels lack dynamic arrest for generalized volume fractions well above 1; much higher than the liquid-glass transition observed in larger ULC particles or stiffer microgels [1]. Their linear rheological response shows similarities with the response of star-like micelles [2]. The plateau modulus, G_P, and the yield stress, σ_y show weaker concentration dependence (orange stars) compared to the regular microgels (synthesized with 5 mol% BIS) whereas undergo a solid-liquid transition at much higher shear strain amplitudes; ULC particles form less fragile networks. From large amplitude oscillatory shear, (LAOS) performed at different frequencies we observed a strain thinning behavior; (decrease of G', G'' with shear strain).

The lack of G'' peak in LAOS indicates weak interpenetration of pNIPAM microgels [3]. The observed behaviour is not reproduced by microgels with the same softness (0 mol%) and different sizes (R = 130 and 375 nm) and by microgels with the same size and different softness. Furthermore, from the SAXS data, we see a decrease in nearest neighbour distance, NND as ζ increases. These findings offer insights into the role of softness in the rheology of small colloids.

Turbidity measurements reveal that suspensions remain transparent for all studied concentrations at room temperature and become milky as temperature increases making this system interesting also for applications, i.e., paints and coatings.

Keywords: Rheology, Microgels, Softness

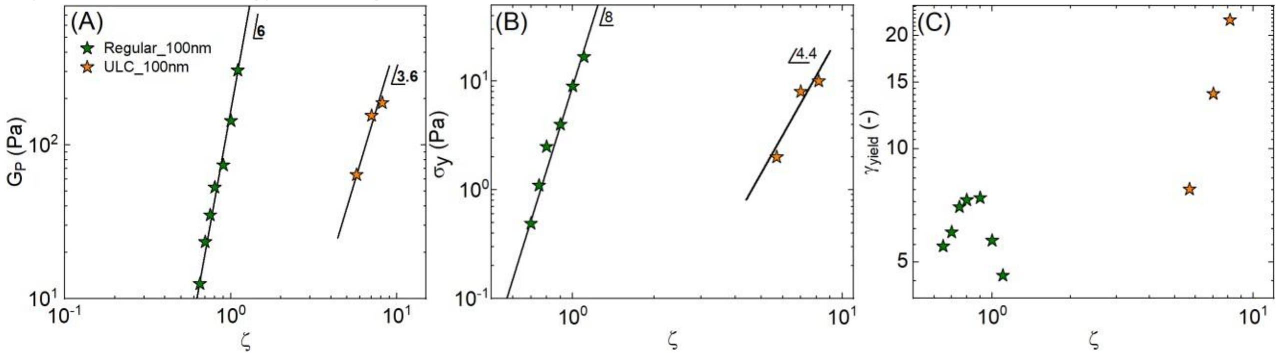

Figure 1. *(A) Plateau modulus, (B) yield stress, and (C) yield strain versus generalized volume fraction, ζ, for: ULC with radius 100 nm (orange stars) and 5 mol% crosslinked with radius 100 nm (green stars).*

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Tuning the structure and dynamics of colloidal gels with polymer brush coatings

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Colloidal depletion gels are self-assembling soft matter systems with complex mechanical behavior. Their structure and rheology can be tuned by adjusting three steady-state variables: particle volume fraction, attraction strength, and attraction range. In this study, we use integrated experimental, computational, and theoretical efforts to introduce a fourth parameter for tuning particle connectivity and dynamics via polymer brush interactions.

In model experimental colloidal gels the particles are coated in a thin polymer brush layer to produce proper steric stabilization. When enough salt is added to screen electrostatic interactions, sufficiently dense surface brushes will produce a rigid barrier that prevents surface-to-surface contacts. This ensures that the colloid-colloid interactions in the system are dominated by depletion. In this study, we find that reducing the amount of monomer used during the polymer brush synthesis step is enough to significantly alter particle level interactions. We systematically compare the use of high and low monomer concentrations for surface brush synthesis across a range of depletant and salt concentrations. The results demonstrate that low monomer concentration consistently produces more restricted particle dynamics. These systems readily produce stringier networks that stabilize at an average contact number ~3 instead of 6. This suggests that significant changes in brush-brush interactions can be controlled with a simple change to the polymer brush synthesis step.

We successfully mimic this phenomenon in simulation by adding a 3-body angular rigidity parameter to standard pairwise particle interactions. In this way, we approximate complex brush-brush interactions as a comparatively simple multi-body effect. These simulation data further support the relationship between monomer concentration and the final brush-brush interactions. Together, our results suggest that the monomer concentration used in surface brush synthesis is an effective knob for tuning gel structure and rheology.

Keywords: colloidal gels, polymer brush, depletion gels, microscopic interactions, central and non-central forces, gel elasticity

Work Hardening in Colloidal Crystals

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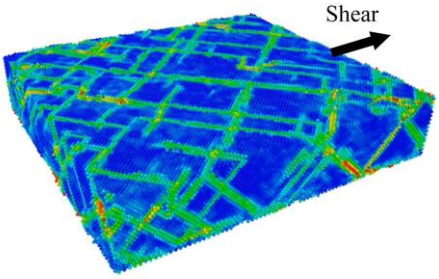
Colloidal crystals exhibit a rich behavior that is in many ways analogous to their atomic counterparts: they have the same crystal structures; they undergo the same phase transitions; and they possess the same crystallographic defects. In contrast to these structural properties, the mechanical properties of colloidal crystals are quite distinct from those of atomic systems. For example, unlike in atomic systems, the elasticity of hard-sphere colloidal crystals is purely entropic; as a result, they are so soft that they can be melted just by stirring. We use confocal microscopy to show that hard-sphere colloidal crystals exhibit work hardening, where they become stronger when subjected to increasing plastic deformation [1]. Their strength increases with dislocation density, and, remarkably, ultimately follows the classic Taylor scaling behavior for atomic materials, even though hard-sphere interactions lack the complexity of atomic interactions. This striking resemblance between colloidal and atomic crystals, despite the many orders of magnitude difference in particle size and shear modulus, demonstrates the universality of work hardening.

Keywords: Colloidal crystals, plastic flow, dislocation dynamics



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Force cessation in microrheology of hard colloids: Simulations and theory

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In active microrheology, a colloidal tracer is pulled through a soft matter system, revealing its mechanical properties at the microscopic scale. This has been accomplished experimentally and studied with theory and simulations mainly in the stationary regime, where a constant force is applied and the velocity is studied, or the tracer is trapped and dragged at constant velocity [1,2]. In this work we focus on the study of force cessation, i.e. what happens when the force is suddenly switched off [3]. For this case, a dense suspension of Brownian spheres is considered with a model based on the mode coupling theory, and simulations with Langevin dynamics.

The viscoelasticity of the system implies a non-trivial response of the system upon releasing the external force: the tracer moves back a distance that shows a non- monotonic dependence on the external force (see Fig. 1). This recoil amplitude increases with the bath density (elastic vs. viscous character), and with the tracer size. The theory is developed for time-dependent forces, containing the schematic ingredients to capture the phenomenology observed in the simulations. Linear response theory can be used to rationalize the overall behaviour for small forces, and the competition between elastic and plastic effects determines the nonlinear recoil.

Keywords: Microrheology, force cessation, tracer recoil, linear response theory.

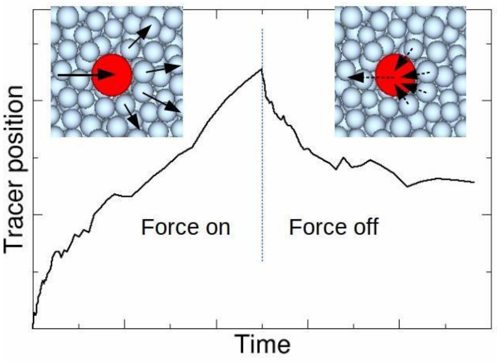

Figure 1. *Schematic representation of the phenomenology.*

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Optothermal growth of 2D colloidal quasicrystals

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We have exploited the thermophoretic drift induced by an infrared laser on a binary colloidal mixture strictly confined in 2D using a 5 mm thick cell [1] to generate close packed structures that effectively mimic a two-dimensional system of non-additive hard disks.

By tuning the mixture stoichiometry - which remains spatially uniform during the optothermal assembly process because the thermophoretic velocity does not depend on the particle size, see Fig. 1 - we managed to obtain 12-fold symmetric quasi-crystals theoretically predicted by equilibrium numerical simulations. No evidence was however found of a 8-fold quasicrystal phase, also predicted to occur in a narrow region of the phase diagram.

Brownian dynamics simulations, where the aggregation of a hard-sphere binary mixture is driven by an external force akin to the optothermal excitation we use, generate structures in agreement with the equilibrium state diagram in Ref. [2], if exception is made of the 8-fold quasicrystal that seems to be dynamically hindered by the occurrence of long-lived metastable phases.

Keywords: hard-sphere mixtures, quasicrystals, thermophoresis, optothermal manipulation.

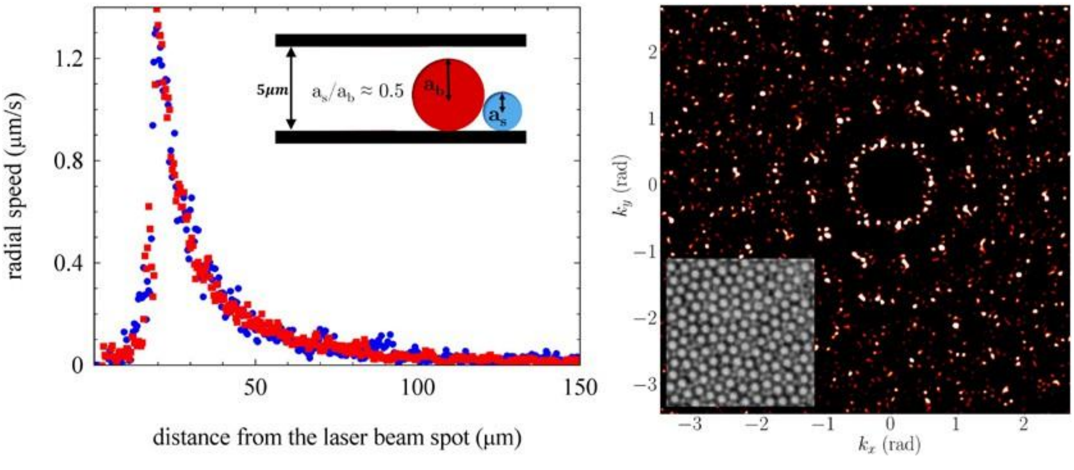

Figure 1. *Left: Radial thermophoretic speed distribution for the two species, with a sketch of the setup. Right: Quasi-crystalline Structure factor of the big particles calculated from the experimental distribution in the (nset.*

Acknowledgements: We acknowledge the financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, of the Italian Ministry of University and Research (MUR), funded by the European Union—NextGenerationEU—Project Title "Thermal Forces in Confined Fluids and Soft Solids"—CUP J53D23001310006

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Data Driven Inference of Colloidal Interactions

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The collective behavior of many-body microscale systems in soft matter and biology is driven by the complex interactions between their constituents. These forces are essential for the emergence of structures and phenomena, and their understanding is a prerequisite for advancing practical applications in areas from materials design to biotechnology and medicine. Colloidal particles move under the influence of thermal fluctuations, mutual interactions, hydrodynamics and sometimes external fields and activity. We propose a toolset to unravel and quantify all these phenomena non-invasively from colloidal trajectories.

Following the core idea developed in [1], we combine linear algebra and information theory, along with model selection criteria, to develop an efficient algorithm for inferring interactions from Brownian trajectories [2]. We validate our method on both passive and active 3D systems simulated using Brownian dynamics with hydrodynamics. We show that we are able to get very good quantitative agreements between the exact and inferred hydrodynamic couplings as well as the self-activity and pairwise interactions.

We further discuss how our method could be combined with 3D trajectories from in-line holographic microscopy using novel contrasts and thresholds [3-4].

Keywords: In-line Holographic microscopy, data driven inference, colloidal interactions, hydrodynamics, activity

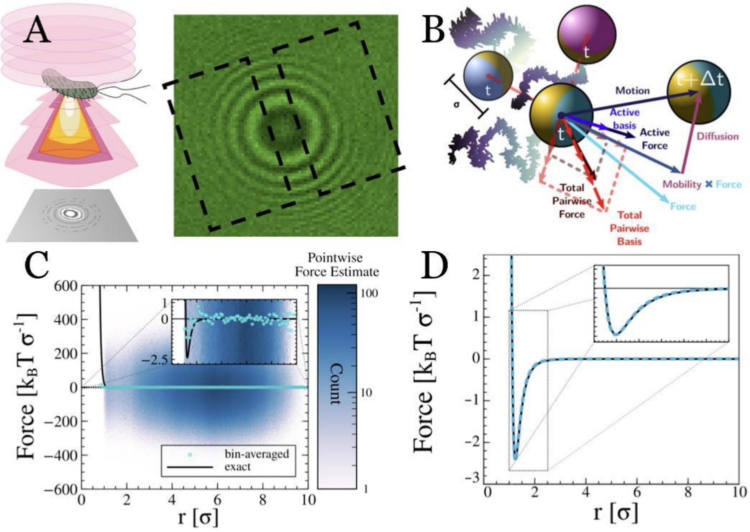

Figure 1. *Illustration of central elements of our approach. A. Schematic of in-line holographic microscopy with an experimental hologram of a metal-dielectric Janus particle. B. Schematic of trajectories in a Brownian dynamics simulation. C. Apparent forces, calculated as Motion/(Δt Mobility), and binned averages (light-blue points). D. Inferred force curves from trajectories of a system of 64 passive Lennard-Jones particles with hydrodynamic coupling.*

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Dynamics and phase behaviour of quasi - 2D dispersions

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Dispersions of globular proteins or colloids with competing short-range attractive (SA) and long-range repulsive (LR) interactions have a rich phase behavior with different cluster phases. While three-dimensional SALR dispersions have been intensely studied also regarding their cluster dynamics [1], less is known about quasi-two-dimensional (Q2D) dispersions where the particles form a planar monolayer inside a bulk fluid.

Using mesoscale simulations without and with hydrodynamic interactions (HI, we have determined the phase behavior and clustering properties of a generic Q2D model where the Brownian particles interact directly by short-range generalized Lenard-Jones and long-range repulsive screened Coulomb forces [2]. The Q2D phases resemble those in three dimensions, but are different in their microstructure showing different levels of hexagonal ordering. With decreasing temperature, the cluster morphology crosses over from disk-like shapes in an equilibrium cluster (EC) phase to double-stranded anisotropic hexagonal clusters in a cluster-percolated (CP) gel phase. Indicators have been identified signaling the transition from a high-temperature dispersed fluid (DF) phase to the lower-temperature equilibrium cluster phase. Furthermore, we have uncovered the dynamics of Q2D – SALR systems including self-diffusion with its non-Gaussian statistics [3]. The interplay of Q2D motion and HI causes anomalously enhanced collective diffusion at small wavenumbers *q* related to out-of-plane fluid backflow. The spatio-temporal buildup of inter-proteins HI by vorticity diffusion and sound is revealed from time-resolved hydrodynamic and velocity (current) autocorrelation functions [3].

Keywords: Quasi – 2D dispersions, dynamics, phases, mesoscale simulations

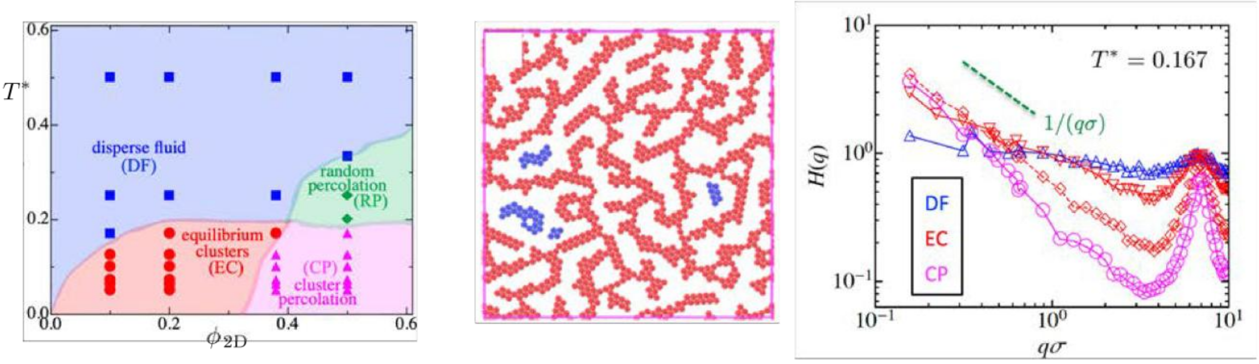

Figure 1. *Left: Phase diagram of Q2D - SALR dispersion. Middle: Simulation snapshot of a cluster - percolated Q2D system. Right: Hydrodynamic function H(q) of indicated Q2D phases.*

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Probabilistic memory outperforms deterministic memory in a Szilard engine with restrictions

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Information engines have garnered significant attention for their potential to harness power and extract work, with recent experiments and theoretical studies shedding light on these concepts. In the classical Szilard engine, a Maxwell demon makes perfect measurements and can extract work equal to the stored information. However, real-world systems often face structural limitations that render some observations ambiguous, hindering work extraction. We explore the implications of such ambiguity in a Szilard engine with a structured, two-pronged divider that introduces an ambiguous region where observations are not useful for work extraction. Using feedback optical tweezers to manipulate a colloidal particle in water, we investigate the efficiency of deterministic and probabilistic memory for work extraction. Our findings reveal that a deterministic two-state memory results in less work extraction than a classical Szilard engine, while a three-state memory can match the coarse graining in the work-extraction medium [1]. In accordance with the second law, operating the memory and work medium at the same bath temperature yields no net gain, due to the high cost of memory. Raising the effective temperature of the work medium can offset this cost, but probabilistic memory can achieve a net positive output at lower increased temperatures than deterministic memory. This research highlights the intricate relationships among system restrictions, resource utilization, and optimal performance, demonstrating that probabilistic memory can outperform deterministic memory in information engines with structural limitations, leading to more efficient information engines in practical settings.

Keywords: Szilard engine, Information encoding, Optical tweezers.

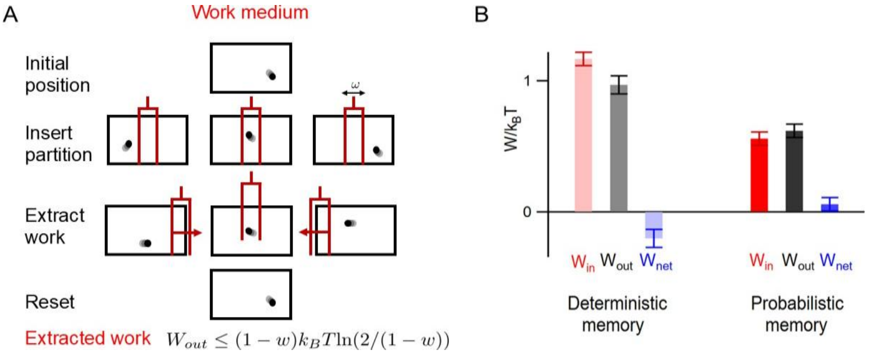

Figure 1. *We demonstrate the advantage of using a probabilistic memory encoding for our modified Szilard engine.* ***A.*** *Inserting a two-pronged divider into the Szilard work medium creates a restricted region (width w) in the middle, which is not useful for work extraction. The rest of the region with width* $(1-w)$ *allows a maximum work output of* $W_{\text{out}} = (1-w)\, k_BT\ln(1-w)$. ***B.*** *For* $w = 0.3$, *and temperature ratio of 1.4 between the work and the memory medium, the cost of memory* W_{in} *is higher than extracted work* W_{out} *in deterministic memory encoding, resulting in negative work output* W_{out}. *However, using probabilistic encoding lowers the memory cost below the output, with positive gain.*

Acknowledgements: We would like to thank Susanne Still and Dorian Daimer for their theoretical insights. This work is supported by FQXi, and NSERC Discovery grants.

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Stochastic size control of self-assembled filaments

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Controlling the size and shape of self-assembled structures is a fundamental challenge in self-assembly, and is highly relevant in material design and biology [1]. This challenge is especially prevalent in one-dimensional structures (filaments), where size control cannot be achieved by balancing surface and bulk contributions to the free energy.

Here, we demonstrate that careful use of programmable, "semi-addressable" binding interactions [2-3] lets us economically assemble filaments of user-defined length. We show that the achievable filament lengths are independent of the size or number of the constituent particles, and that varying the number of individually addressable particle species allows us to explore fundamental design trade-offs between assembly quality (spread in size) and cost (number of particle species, assembly time).

Our work reveals that size control of filaments is possible in thermal equilibrium exclusively by exploiting short-ranged binding interactions in a way that is immediately applicable to a broad range of programmable self-assembly platforms, from macromolecular polymers to DNA origami and beyond.

Keywords: self-limiting assembly, programmable interactions, semi-addressable regime

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A closer look on bicelles using scattering, ab initio modelling and molecular dynamics

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Bicelles are self-assembled lipid objects composed of long-chain and short-chain lipids or detergents that under certain conditions may form disk-like structures in water solutions. Their detailed morphology and overall size depend on numerous parameters where one of the most important ones being the molar ratio of the constituents (q_{eff}). Although there is general consensus in relation to the overall properties of systems like DMPC/DHPC, many scattering, NMR or real-space studies report somewhat contradicting results about their exact morphology.

In an effort to elucidate fine details of bicellar structure, we employed a combination of solution small angle neutron and X-ray scattering (SANS/SAXS). Going beyond the simple use of form factors for the analysis of the scattering data. we developed a stochastic methodology for the generation of *ab initio* bicelle shape reconstructions under concurrent SANS and SAXS constraints. We report on the effects of lipid mixing, overall geometric parameters and aggregation as a function of q_{eff}. Additionally, we compare the findings of our scattering experiments with results from extensive coarse grained molecular dynamics simulations (MARTINI force field) of DMPC/DHPC self-assembly as a function of q_{eff}.

We argue that this integrated experimental/simulation investigation reveals valuable and detailed information concerning bicelle morphology especially in relation to modeling approaches involving only analytic form factors, that will contribute to the SANS/SAXS modelling of peripheral or integral membrane proteins in interaction with such membrane mimics.

Keywords: icelles, SANS, SAXS, ab initio, molecular dynamics

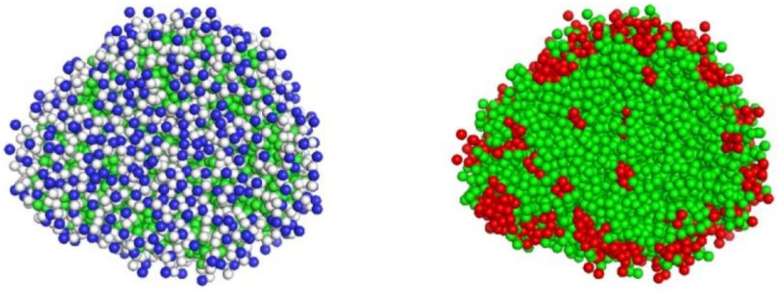

Figure 1. *Representative bicelle structure as revealed by MD simulations. On the right DMPC/DHPC molecules colored green and red respectively.*

Making and Breaking Colloidal Gels by Mechanochemistry

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Mechanical forces are critical in shaping biological processes and maintaining the structure and function of organisms at various levels: from cellular to organ systems. These forces play essential roles in a range of biological functions, including tissue development, wound healing, cell signaling, and the maintenance of homeostasis. Soft biological tissues are composed of macromolecular and low-molecular components, containing covalent and non-covalent crosslinks, and are assembled in a modular way exhibiting different hierarchy levels.[1] Such hydrogel-like materials often exhibit hysteresis effects and non-linearity of their mechanical properties, which is essential to functions like adaptability and time-programming.

Aqueous colloidal gels may serve as perfect model systems to understand many fundamental aspects of the mechano-chemistry, mechano-responsiveness and mechano-actuation because their properties can be tailored by precision synthesis methods and they can be used as colloidal building blocks to fabricate hierarchically structured soft materials in a modular way.

This contribution will focus on chemical design of microgels using mechanochemical polymerizations[2] and behavior of mechano-responsive colloidal gels in force fields.[3] Synthesis approaches to obtain mechano-responsive colloidal gels exhibiting weak covalent (disulfide, diselenide) and non-covalent (host-guest complexes, ionic bonds or hydrogen bonds) crosslinks will be described.[4-7]

We demonstrate that obtained colloidal gels exhibit reversible temperature- or pH-triggered swelling/deswelling in aqueous solutions. Upon application of mechanical force, colloidal gels show interesting properties like self-repair, on-demand degradation, ROS scavenging and controlled release of biomolecules.[8-10]

Keywords: microgels, mechanochemistry, mechano-responsiveness

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Optimizing ATP-like energy delivery in synthetic nanomachines via path reweighting and automatic differentiation

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ATP and other chemically charged molecules provide an incredibly efficient mode for delivering energy to motor proteins and other biological nanomachines, allowing them to do work and perform tasks. While it is now possible to engineer complex nanostructures out of synthetic building blocks, we lack the ability to endow them with machine-like functionality in part because efficiently delivering energy where and when it is needed remains a challenge. In order to take full advantage of our engineering capabilities we need efficient and reliable tools that let us connect the particle level design attributes to the functional and dynamic target behavior of the assembled system.

I will show how to combine path reweighting, a tool for recovering the correct properties from a modified potential energy surface without having to re-simulate the whole system, and automatic differentiation, a set of tools to compute derivatives of programs, in order to compute gradients of dynamical observables like transition rates without having to store and differentiate through the whole simulation trajectory. This makes it possible to formulate the task of achieving some desired functionality as the solution to an optimization problem, which can then be solved using modern gradient based optimizers. I will go on to show how this framework can be used to optimize the transfer of energy between a charged fuel source and an uncharged nanomachine. In this way we can further improve the performance, power and occupation enhancement compared to the baseline [1].

Keywords: self-assembly, inverse design, kinetics, path reweighting, automatic differentiation

References

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Unravelling and controlling crystallization pathways of colloidal cube superstructures

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Recent advancements in anisotropic particle synthesis and self-assembly have enabled the formation of diverse superstructures and crystalline materials with novel mechanical, optical, and electronic properties. However, the precise mechanisms governing the self-assembly of anisotropic particles and their arrangement into final superstructures remain elusive at the single-particle level. Without a fundamental understanding of the self-assembly process, our ability to control and design these assemblies remains limited, constraining the full potential of emerging functional materials.

Here, we investigate the crystallization pathways leading to different final structures, namely square and Λ_1, in anisotropic colloidal 'superballs', i.e. cubes with rounded corners[1] under the influence of critical Casimir forces[2,3]. The critical Casimir force provides precise tuning of the interparticle attraction via temperature allowing in- and out-of-equilibrium assembly. Using high-speed confocal microscopy and image analysis routines, we investigate different attraction strengths and cube concentrations and follow the particle dynamics, interactions, and superstructure formation in-situ on a single-particle level. We find that the final crystalline structures and cluster morphology are highly dependent on the pathway used to modulate the attraction strength. Additionally, we unravel the pathways for achieving dense, large clusters as well as thin and thick branched network structures with controlled cubic and Λ_1 ordering. We finally demonstrate how by carefully tuning the attraction strength and assembly pathway, one can precisely control the formation of ordered crystals, defect-rich structures, or disordered network-like assemblies. Our findings provides fundamental insights into the forces and pathways governing the order and disorder formation during the self-assembly of anisotropic (nano)particle superstructures, contributing to the rational design of functional materials.

Keywords: Colloidal superballs, crystallization, critical Casimir force, self-assembly, anisotropy

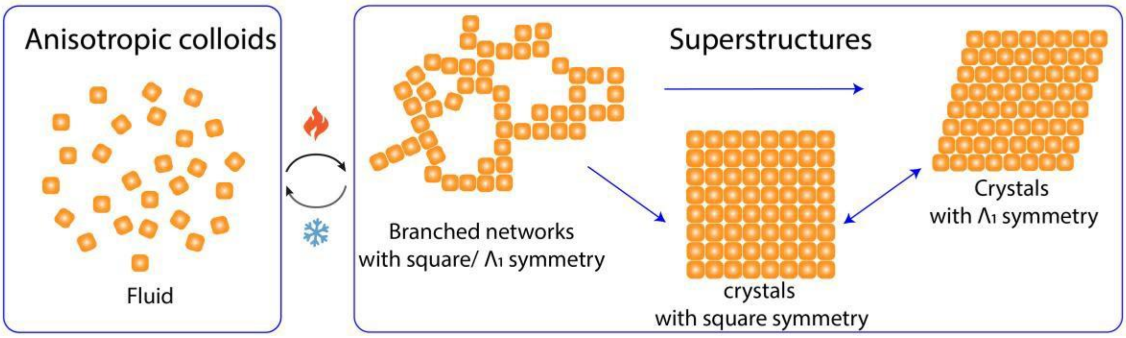

Figure 1. *Schematic representation of 2D crystallization of colloidal cubes in presence of critical Casimir forces.*

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Real-space investigation of aging dynamics in Laponite colloidal gels

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Aging, a slow structural relaxation process, is a universal phenomenon in systems with limited particle mobility, such as glasses and gels. Recent studies have highlighted key differences in aging behavior between these glassy and gel states [1]. However, the mesoscale structural evolution of gels under different interaction strengths is still poorly understood.

Here, we explore the aging dynamics of charged colloidal Laponite by systematically tuning the interparticle interactions from repulsive to attractive through the salt addition. Direct imaging using both fluorescence labeling reveals that the structural evolution upon aging changes with salt addition along the arrow in the phase diagram (Fig. 1a) [2]. It is shown that at low salt concentrations, where repulsion dominates, the suspension undergoes homogeneous gelation. In contrast, at high salt concentrations, aggregation transitions from a coarse to a fine, heterogeneous structure (Fig. 1b). Additionally, we perform particle tracking analysis to capture the microscopic dynamics of aging, revealing changes in the local rheology in Laponite-rich and -poor phases, respectively (Fig. 1c). In the colloid-rich phase, unlike in the colloid-poor phase, the distribution of displacement Δx becomes non-Gaussian, suggesting spatial inhomogeneity. In our presentation, we will discuss the difference in the structural evolution upon aging due to a competition between phase separation and the glass transition, which arises depending on the interactions between the particles.

Keywords: Laponite, colloidal gel, aging, real-space observation, particle tracking

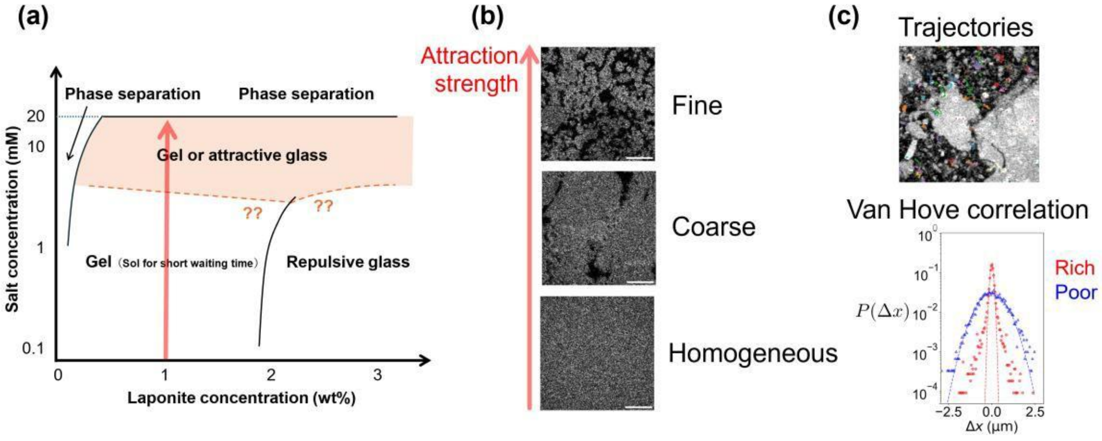

Figure 1. *(a) Phase diagram of Laponite suspensions* [2]. *(b) Real-space fluorescence images showing different aging structures: homogeneous, coarse, and fine aggregation. (c) Micro-rheology measurements by particle tracking*

Acknowledgements: We thank Prof. Sooyeon Kim and Prof. Yuichi Taniguchi (Kyoto University) for valuable discussions and technical support.

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Intelligent Microrobots Made from Colloidal Assemblies

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Colloidal scale robotic systems offer exciting opportunities for intelligent behavior without relying on conventional computational hardware. Unlike macroscale robots, micro- and nanorobots at the colloidal level achieve sensing, control, and adaptation through their material composition and physical design. In this talk, I will present two recent colloidal assembly strategies for engineering colloids with programmable structures and responsive functionalities, aimed at applications in biomedicine and environmental sustainability.

First, we harness evaporation-driven self-assembly to construct colloidal assemblies with tunable geometries and multi-compartment architectures, enabling controlled motion and cargo release [1,2]. Second, we employ capillarity-assisted particle assembly to achieve modular integration of colloidal building blocks with high spatial precision. This technique supports the incorporation of distinct liquid compartments and functional components, allowing for autonomous motion and localized sensing [3,4].

Together, these approaches establish a versatile colloidal platform for embedding multiple functional components and various responsive mechanisms within a single microsystem. By exploiting colloidal assembly approaches, we aim to develop intelligent colloidal materials capable of performing complex tasks in dynamic environments.

Keywords: Evaporation-Driven Self-Assembly, Capillary Assembly, Microrobots

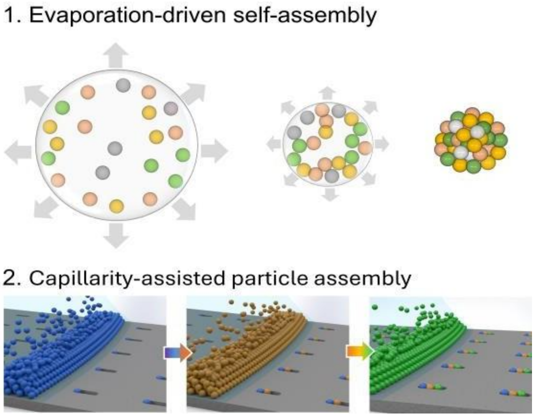

Figure 1. *Schematic picture of colloid assembly strategies.*

Acknowledgements: M. Hu thanks the financial support from Swiss National Science Foundation (Ambizione Grant, No. 216253).

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Dielectrophoretic directed assembly of quantum plates for quantum color conversion in micro-displays

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Building competitive color conversion pixels for micro-displays made of semiconductor nanocrystals requires reaching a deposition thickness high enough to absorb all the blue light from the backlight unit (see Figure 1, center). In the case of dielectrophoretic directed assembly of such nanocrystals, modeling and simulations helped understand what the intrinsic limitations of the process are, and were used to propose new assembly routes.

A theoretical model of dielectrophoretic interactions between polarizable nano-spheres and an electrostatically patterned substrate has been developed. Monte Carlo simulations have been run using this model to rationalize the effects of parameters driving the dielectrophoretic directed assembly and to find optimal deposition conditions for reaching a maximal thickness of nanocrystal pixels. Experiments with CdSe quantum plates and with alumina spheres embedding quantum plates (micro-pearls) have been carried out and compared to the model.

Modeling and simulations reveal that the directed assembly of semiconductor nanocrystals is limited essentially by the small object size, which sets the maximum dielectrophoretic force they can undergo. They indicate that using larger objects loaded with quantum dots or plates should allow reaching unprecedented assembly heights, but also induces an undesired lateral extension of the assembly. This trade-off has been illustrated with diagrams in the parameter space and confirmed experimentally with micro-pearls.

Keywords: modeling, experiments, nanoxerography, dielectrophoresis, assembly, quantum dots.

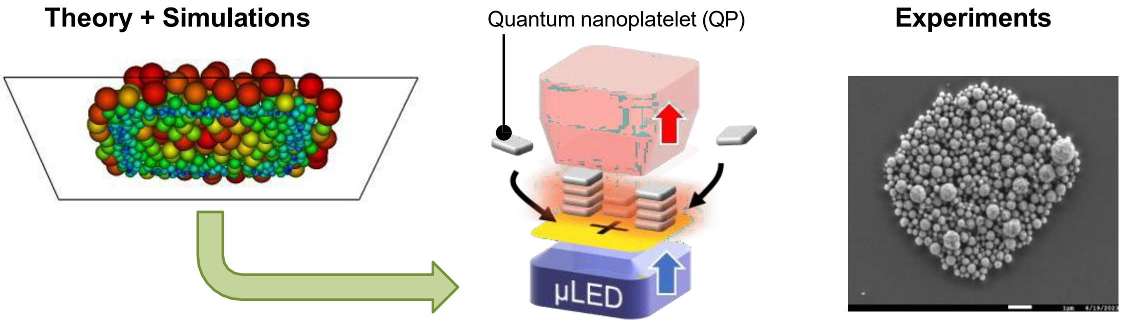

Figure 1. *Center: general structure of a quantum color convertor in a micro-LED display (here, blue light is converted to red by the quantum plates assembled above the micro-LED). Left: Monte Carlo simulation of a polydisperse micro- pearl assembly (view from blow the substrate). Right: experimental realization of the dielectrophoretic assembly of micro-pearls on a 5 µm pixel.*

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Thursday 2nd October 2025

I. Interfaces, surfaces, membranes, emulsions

(Room 2)

Elastic Microphase Separation Produces Bicontinuous Materials

Carla Fernández-Rico[1], Sanjay Schreiber[1], Hamza Oudich[2], Charlotta Lorenz[1], Alba Sicher[1], Tianqi Sai[1], Viola Bauernfeind[3], Stefanie Heyden[1], Pietro Carrara[2], Laura De Lorenzis[2], Robert W Style[1], Eric R Dufresne[1,4]

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Phase separation is a fascinating physical process that is not only responsible for the internal organization of living cells but also a promising tool for structuring materials. The central challenge in making meso-structured materials via phase separation is the lack of structural control at length scales beyond the macromolecular scale.

In this talk, I will introduce Elastic MicroPhase Separation (EMPS) as a route to create highly correlated and bicontinuous structures in the scale of hundreds of nanometers (see Fig.1). The essential idea of our approach is simple; we counter the thermodynamic forces that drive phase separation with elastic stresses in the host matrix [1,2]. In this way, we can tune the size and morphology of the structures by changing the mechanical properties of the matrix. Analysis of the microstructure, phase equilibria, and kinetics suggests that these systems emerge through a unique thermodynamic pathway, featuring aspects of both nucleation and growth and spinodal decomposition. We demonstrate the potential our approach by toughening polymeric materials, and making bi-continuous structures with controlled structural and anisotropic gradients.

Keywords: Phase separation, bicontinuous structures, elastomers

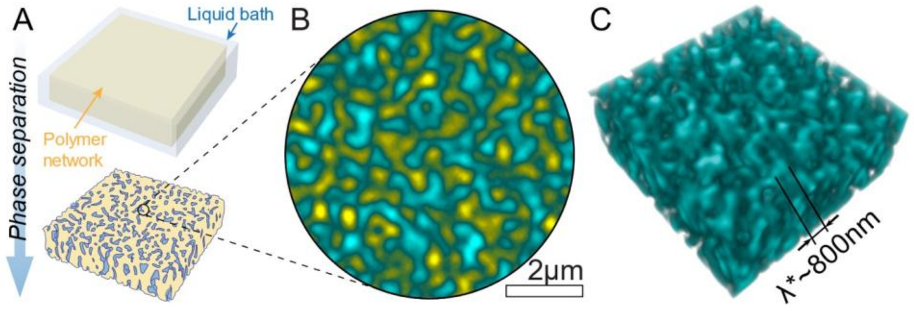

***Figure 1**: Elastic microphase separation produces bicontinuous structures. (A) Schematic of the synthesis process. (B,C) Confocal 2D and 3D snapshots of the bicontinuous structure obtained after phase separation.*

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Understanding the stability of Pickering emulsions using on-chip microfluidics

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Particle-stabilized emulsions, commonly referred to as Pickering emulsions, offer superior stability, and functional versatility, compared to conventional surfactant-stabilized emulsions. While the majority of the work in this field has focused on densely covered Pickering emulsions, such emulsions are known to retain their exceptional stability even when the interfaces are sparsely covered with particles. Here, I will present our latest findings regarding the formation, dynamics, and stability of poorly covered model Pickering emulsions using a microfluidic platform, enabling precise design, production, and systematic analysis. I will show that the formed Pickering emulsions remain highly stable, over at least 12 hours, even with a surface area coverage below 3%. By directly visualizing the droplet interface at various stages, the exceptional stability is attributed to the highly spatially heterogeneous distribution of the adsorbed particles which exclusively form particle bridges at the contact point between the droplets. Remarkably, these bridges are assembled in the form of crowns between the droplet interfaces, as visualized by confocal microscopy. Lastly, I will discuss the different forces present during emulsification and how the assembly behavior of the adsorbed particles is dominated by hydrodynamic forces leading to a non-uniform particle distribution, corroborated by numerical simulations [1]. In conclusion, our work provides an easy-to-access, controlled lab-on-a-chip platform to study Pickering emulsions, and gives important insights about the production and dynamics of Pickering emulsions via preferential interfacial localization of particles.

Keywords: Pickering emulsions, microfluidics, droplet coalescences, stabilization

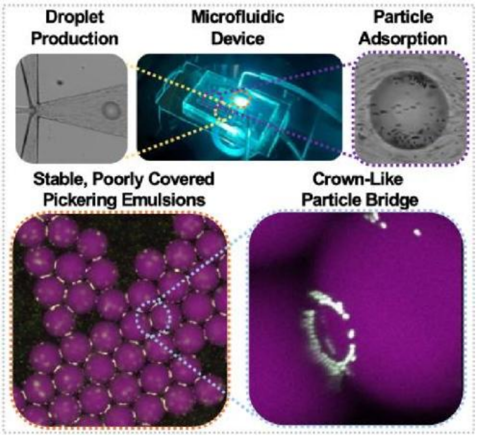

Figure 1. *Working principle of microfluidic device and stabilization mechanism of poorly covered Pickering emulsions.*

Acknowledgements: This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No. 956248.

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Controlling the partitioning of binary particle mixtures in bijels for high-capacity lithium-ion batteries

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Lithium-ion batteries (LIBs) are essential for electric vehicles, portable electronics, and largescale energy storage systems. However, the tradeoff between energy and power density hinders LIBs from simultaneously achieving high capacity and rapid charging speeds [1]. This tradeoff can be overcome by integrating high-capacity electrode materials into bicontinuous interfacially jammed emulsion gels (bijels) with sub-micron domains.

Such nano-structured bijels can be synthesized using either surfactant or covalently functionalized silica nanoparticles [2-3]. Here, we investigate for the first time the combination of both surfactant and covalent modifications. We hypothesize that surfactant functionalization enables bijel stabilization, while covalent functionalization facilitate battery particle integration.

To validate this hypothesis, we analyze both particles types and bijels via zeta potential measurement (ζ_{pot}), dynamic light scattering (DLS), titration, Fourier-transform infrared spectroscopy (FTIR), and confocal laser scanning microscopy (CLSM). FTIR confirms the gradual control over battery particle functionalization via silane chemistry. This controlled functionalization is crucial for maintaining colloidal stability, as evidenced by ζ_{pot}, DLS, and titration data. Moreover, CLSM visualizes how controlling particle functionalization affects the partitioning of both particles in the bijels. The combined results of this study pave the way toward engineering bijel batteries with both high energy and power densities.

Keywords: Bijels, Surfactant adsorption, Lithium-ion battery

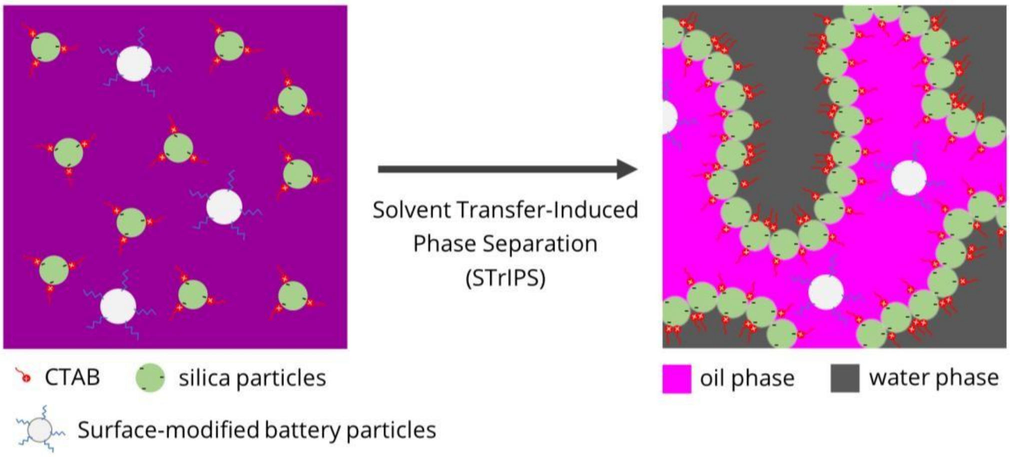

Figure 1. *Schematic illustration of the selective adsorption of surfactant during the formation of a particle-stabilized bicontinuous emulsion.*

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Structure and polymer dynamics in one component polymer nanocomposites (OCNC)

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Structure and dynamics of polymer chains grafted to a nanoparticle (NP) surface in one component nanocomposites (OCNC) are investigated by small angle scattering (SAXS, SANS) and neutron spin echo (NSE) [1]. The OCNC were realized by self-assembly of block-copolymers and subsequent crosslinking of the core. The sizes of the resulting NPs were narrowly distributed. Owing to equal core and shell volumes the melt structure is that of a concentrated colloidal dispersion of cores. The melt structure could be reasonably well described by a Percus-Yevick structure factor. In order to access more deeply the dynamics, three differently labeled materials with labels at the inner- or outer part and the whole graft were studied. The experimental data were evaluated in terms of models allowing for site dependent friction. For this purpose, the Langevin equation containing a friction profile was solved and the dynamic structure factor in terms of its eigenvalues and eigenvectors was compared to the data. Even though the grafting density was low (about 0.3 chains/nm^2), our results show that the monomeric friction increases significantly close to the grafting point and decreases to constant friction in the direction of the chain ends. Furthermore, we demonstrate that dynamic heterogeneity needs to be assumed, in order to describe the experimental spectra (Figure 1). We relate this heterogeneity to the structural peculiarities of the dense core arrangement.

Keywords: polymer dynamics, neutron scattering, nanocomposite

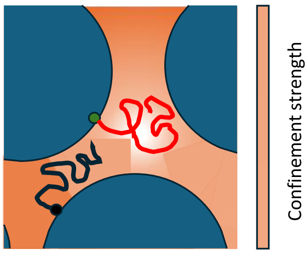

Figure 1. *Heterogeneities for the dynamics of a grafted chain: black chain is more confined than the red one.*

Acknowledgements: We thank Ingo Hoffmann, Lionel Porcar, Olga Matsarskaia and Martin Dulle for their support at the neutron scattering and SAXS experiments.

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Understanding the effect of Hevea brasiliensis latex particle size on interfacial and mechanical properties

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Latex, obtained by tapping of the bark of Hevea brasiliensis trees is a colloidal suspension of various micrometric objects, mainly composed of rubber particles (RP) which contain cis-1,4-polyisoprene chains. Hevea latex is the only commercial source of natural rubber (NR), a strategic and essential raw material used for automotive, medical and consumer applications. RP are composed of a hydrophobic cis-1,4-polyisoprene core surrounded by a monolayer membrane (lipids-proteins) exhibit a bimodal size distribution, named small rubber particles (SRP, diameter ~ 0.05-0.4 µm) and large rubber particles (LRP, diameter <1µm). In addition, according to their size, the biochemical composition varies [1]. We will show how RP size and their associated biochemical composition influence the natural coagulation process (without acid) and the final mechanical properties of rubber sheets. The originality of the study lies in its multi-scale and multidisciplinary approaches, involving both the biochemical analysis of native RP and their self-organization in the liquid state, and the mechanical characterization of dry rubber sheets. Firstly, using a Langmuir trough, the adsorption kinetics and the interfacial film formation were followed by complementary techniques such as ellipsometry, tensiometry, interfacial rheology and Brewster angle microscopy for both particle sizes. These methods enabled us to observe the initial stages of coagulation (disruption) and the reorganization of RP components, subsequently analyzed by atomic force microscopy [2]. Secondly, the interfacial study was linked to the mechanical properties of rubber in its solid form, through uniaxial tensile tests on rubber sheets formed from both particle sizes. This work opens up new prospects for future research in this field by linking molecular processes to the macroscopic mechanical behavior of natural rubber.

Keywords: Natural rubber, Coagulation, Interface measurements, Biochemistry

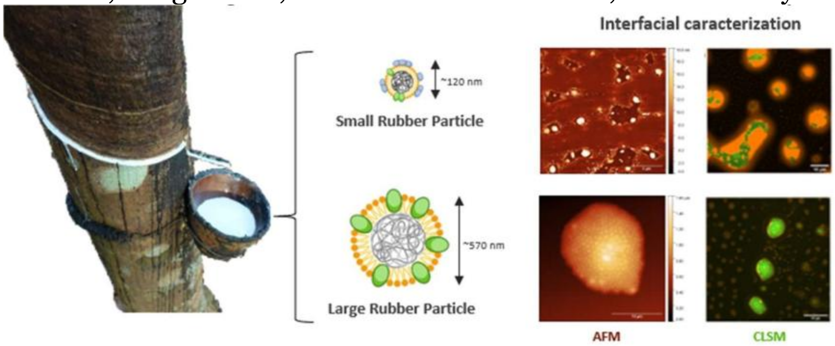

Figure 1. *Schematic diagram of the methodology and results.*

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Temperature-driven mass transport at the nanoscale

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Thermal gradients move matter, causing fluid slip, particles to migrate, selective transport across membranes, and thermoelectric fields to form in ionic fluids. These effects are crucial in energy conversion [1], desalination, microfluidics and biology, but remain poorly understood at the microscopic level hampering the development of new applications. The microscopic origin of these effects is deeply connected to thermo-osmosis, namely the flow of a fluid in presence of a temperature gradient and a confining surface. Indeed, while in macroscopic bulk systems fluid flows are always driven by pressure gradients or external forces, at the microscopic scale, interfacial effects might become relevant and additional mechanisms leading to mass flow are possible. One of these effects is thermo-osmosis.

The first theoretical explanations of thermo-osmosis concern rarefied gases and are based on kinetic theories [2]. In liquids, the adopted phenomenological descriptions rely on macroscopic approaches [3], which cannot be justified when the relevant physical quantities vary on a length scale comparable to the range of interactions, as in the case of surface driven phenomena. Recently, interest in thermo-osmosis has been revived by molecular dynamics simulations aimed at a microscopic understanding of this effect [4].

Stimulated by these findings, the authors proposed a first-principle and unitary theory of thermo-osmosis [5], valid both in the rarefied and in the dense limit, that quantitatively relates the fluid flow to the equilibrium properties of the fluid-wall interface via suitable dynamical correlation functions at equilibrium. To validate our theoretical predictions in a controlled environment, we performed extensive nonequilibrium molecular dynamics simulations for a simple, one-component fluid in a closed channel under a temperature gradient. The comparison between numerical and analytical results is remarkable both in the low and in the high-density regimes, allowing for the quantification of the thermo-osmotic effect given only the inter-molecular interactions [6].

Keywords: thermo-osmosis, thermophoresis, thermal forces, surface interactions, nanofluidics

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Amphiphile-like stabilizers for water-in-water emulsions

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Aqueous two-phase systems or water-in-water (w/w) emulsions constitute a distinct type of colloidal systems in which two immiscible aqueous phases coexist. They are formed from mixtures of hydrophilic macromolecules that are thermodynamically incompatible such as dextran (Dex) and poly(ethylene glycol) (PEG). The capacity to encapsulate active ingredients and regulate substance release, while being composed of fully biocompatible components, holds great potential for application of such systems in food science, encapsulation and drug delivery [1]. However, the stabilization of these peculiar emulsions is much more challenging than for common ones because the interface is not only absent of distinct hydrophobic and hydrophilic regions but is also thicker than that of oil-water systems [2].

We stabilize such w/w emulsions with macromolecular complexes that have affinity for both PEG- and Dex-phases, and therefore, are located at the droplet surface similar to ordinary surfactants at water/oil interfaces. The stabilizing complexes are formed due to 2 :1 inclusions of curcubit[8]uril (CB[8]) with PEG and Dex functionalized with methylviologen (MV) and naphthol (Np), respectively. By finely adjusting the size of the polymers and the grafting ratio with the host groups, we aim at controlling the adsorption kinetics and the strength of the polymer interactions at the interface. This approach enables a systematic investigation of interfacial host-guest complexation as a means of stabilizing w/w emulsions.

Keywords: water-in-water emulsions, host-guest interactions, interfacial complexation

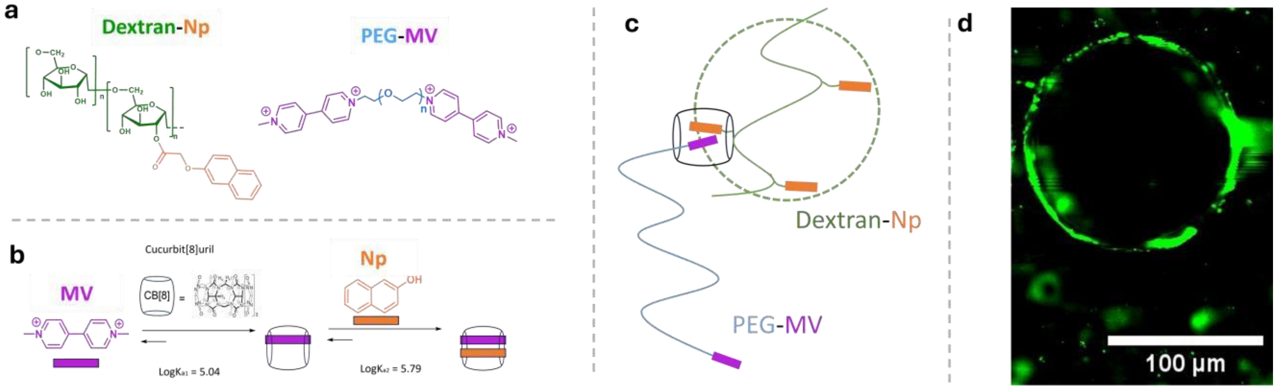

Figure 1. *a) Chemical structures of functionalized Dex and PEG, b) host-guest inclusion formation; c) principle of interfacial complexation in w/w emulsion; d) confocal laser scanning microcopy image of PEG-in-Dex w/w emulsion stabilized by the interfacial complexes using fluorescein-labeled Dextran-Np.*

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How phospholipids stabilize macro and nanoemulsions?

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Delivering an emulsion intravenously for nutrition or drug delivery requires droplets to remain metastable at the sub-micronic scale in high ionic strength conditions. There is a large interfacial area to cover with a surfactant monolayer in these nanoemulsions and the amphiphilic species must be non-toxic. Phospholipids are thus industrially used to meet these constraints. However, their low preferred curvature, which sensitively depends on molecular structures and interactions, is not favorable for stabilizing emulsion droplets. We have investigated this problem to find a rationale for choosing formulation conditions leading to metastable emulsions, based on a fine understanding of interfacial properties and structure.

Four phase diagrams were established for ternary aqueous systems containing either DOPC or POPC as the phospholipid and hexadecane or miglyol 812 as the oil. Droplet interfaces were probed using small-angle neutron scattering and the amount of adsorbed lipid was determined using separation and Raman spectroscopy. The metastability of both nano and macro emulsions was systematically assessed over weeks using light scattering.

We show that a lipid monolayer stabilizes nanoemulsion droplets and display excellent metastability if the preferred curvature is positive and large enough, even without any added charges or at high ionic strengths. In contrast, macroemulsion droplets are stabilized with a lipid multilayer, which should possess a positive preferred curvature but also a good enough interfacial anchorage, which is lost upon increasing the preferred curvature. Overall, we provide a mechanistic description through which we can understand the impact of molecular changes in the formulation on emulsion metastability, through the analysis of the lipid film preferred curvature, layering, and interfacial anchorage. These results demonstrate how a virtuous circle can be established between fundamental soft matter approaches and industrial applications in complex formulations.

Keywords: Parenteral, Emulsion, Self-assembly, Curvature, Metastability

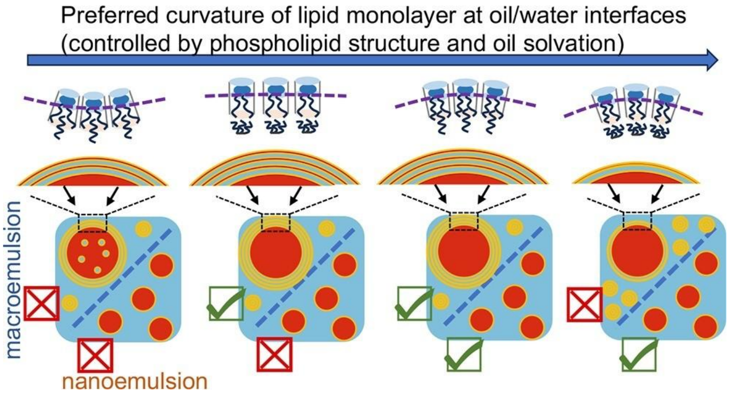

Figure 1. *For Brownian droplets of nanoemulsions, the interface is a phospholipid monolayer. Metastability requires a preferred curvature that is turned sufficiently towards the oil, which can be achieved by selecting carefully the phospholipid and oil of the formulation. When droplets get larger, the metastability barriers have to get stronger to prevent coalescence in the creaming emulsion, which requires a phospholipid multilayer that is only achieved when the preferred curvature is turned towards the oil but not too much.*

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Evaporation Induced Destabilization of Oil-in-Water Emulsion

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Emulsions are widely used in commercial products such as cosmetics, paints, and adhesives [1]. These products are often used as coating layers where drying of the volatile component is inevitable, often leading to coalescence and deformation of the oil droplets [2]. In this work, we present the evaporation-induced destabilization of a single oil-in-water emulsion droplet. The contraction of the air-water interface due to the evaporation of water leads to the vertical compression of the oil droplets. In response to the compression, the droplet flattens in the direction of the compression and expands laterally, ultimately leading to bursting. The area expansion of the oil droplet under compression shows a non-linear behavior and is independent of the initial droplet size. The droplet flattening, however, increases with increasing droplet size. The maximum expansion of the droplet before bursting is found to be independent of the initial droplet size. A morphological investigation of the particulate film at the droplet surface revealed the nucleation of cracks in the lateral surface as the droplet area expands beyond a critical threshold. The cracks propagate towards the top and bottom surface of the droplet under compression as the expansion increases, as shown in the Figure. 1. When the area fraction of the cracks surpasses a critical value, the particulate film ruptures, resulting in the bursting of the oil droplet. Further, the crack area fraction, a critical areal expansion for the crack nucleation, the evolution of the crack area, and the number with the areal expansion are quantified. In addition, the bursting behavior of a droplet in the presence of the nearest neighbor is also discussed in detail.

Keywords: Emulsion, Pickering emulsion, Destabilization, Drying, Colloids

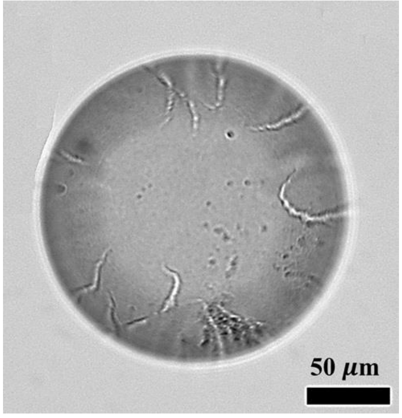

Figure 1*: Bright-field optical microscopy image of a compressed oil droplet with crcaks in the particulate film at the oil-water interface.*

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The role of hydration and electrostatics in salt crystal growth

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Salt crystal growth from supersaturated solutions is a crucial process in both natural environments and industrial applications, yet they remain not fully understood at the molecular scale. Recent research suggests that interfacial phenomena, including water structuring, atomic roughness and surface charge critically influence water transport properties in porous salt crusts [1,2]. Hence, there is fundamental to investigate how these factors impact the crystal growth.

We utilize molecular dynamics (MD) simulations to examine the crystal growth mechanisms of three common salts—NaCl, KCl, and Na_2SO_4—by analyzing their interaction with pre-existing crystal surfaces. Our simulations reveal that ion adsorption on crystal surfaces is driven by a balance of electrostatic interactions and hydration effects, with notable differences between the salts. For NaCl, we found that Na^+ ions preferentially adsorb to the crystal surface, resulting in charge build-up, which subsequently promotes the adsorption of Cl^- ions. KCl shows more balanced adsorption behavior between K^+ and Cl^-, while Na_2SO_4 exhibits strong adsorption of sulfate (SO_4^{2-}) ions, leading to distinct charge layering effects.

Crucially, we identify anomalous crystal growth arising from specific defect topologies such as steps and kinks on NaCl surfaces. These defects significantly alter local adsorption energies, creating favorable sites selectively occupied by ions or water molecules. The strong competition between hydration and electrostatic forces at these defect sites results in the irregular surface structures. These findings offer detailed insights into the molecular mechanisms of salt crystallization and have implications for understanding salt precipitation.

Keywords: Ion adsorption; Hydration; Water transport; Molecular Dynamics

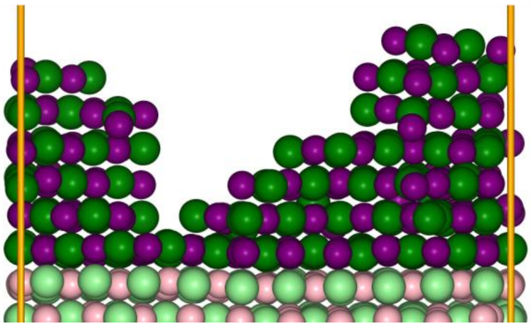

Figure 1. *Side view of a grown NaCl crystal obtained from a supersaturated solution in contact with a planar crystal surface. The atoms belonging to the initial surface are shaded light.*

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Intermittency and dynamical regimes in concentrated emulsions under Rayleigh-Bénard thermal convection

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We present a comprehensive work on thermal convection in emulsions, emphasizing the role of finite-sized droplets. By employing lattice Boltzmann simulations [1], we explore emulsions with varying dispersed phase volume fractions (ϕ), ranging from dilute (Newtonian rheology) to jammed (non-Newtonian yield-stress rheology), within the paradigmatic Rayleigh-Bénard (RB) setup, i.e., confined between two parallel walls at different temperatures under the effect of buoyancy forces; the latter is encoded in the dimensionless Rayleigh number (Ra). In jammed emulsions, sustained thermal convection arises through an intermittent mechanism characterized by intense, short-lived convective "heat bursts" separated by long-lasting conductive periods. This behavior stems from fluidization-rigidity transitions driven by the interplay between yield-stress rheology and plastic activity, leading to emulsion phase inversion induced by droplet coalescence during heat bursts [2]. However, phase inversion is not the only structural change affecting emulsions under convection. Indeed, by exploring the phase diagram Ra vs. ϕ, emulsions may exhibit distinct convection regimes (see Fig. 1). At high values of Ra, breakup-dominated dynamics emerge for low/moderate values of ϕ. In contrast, phase inversion occurs for large values of ϕ only. Both droplet breakup and coalescence significantly alter emulsion rheology [3]. A statistical analysis of the dynamics at the droplet scale helps clarify the observed scenario. This study offers unprecedented insights into the complex interplay between thermal forces, emulsion structure, and rheological properties, bridging gaps in understanding emulsions under buoyancy-driven thermal flows.

Keywords: Emulsions, non-linear rheology, Rayleigh-Bénard thermal convection

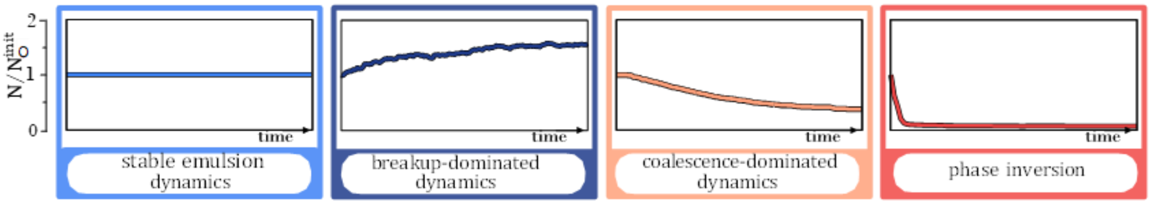

Figure 1. *Summary of dynamical regimes of emulsions under RB thermal convection, resulting from different combinations of ϕ and Ra. The distinction is based on the time evolution of the number of droplets* N *with respect to its initial value* N^{int}*: stable convective regime (no variation of* N*); breakup-dominated dynamics (*N *increases due to breakup events); coalescence-dominated dynamics (*N *decreases due to coalescence events); phase-inverted emulsion.*

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Melting of non-reciprocal solids: how dislocations propel and fission in flowing crystals

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When soft matter is driven out of equilibrium its constituents interact via effective interactions that escape Newton's action-reaction principle. Prominent examples include the hydrodynamic interactions between colloidal particles driven in viscous fluids [1,2], phoretic interactions between chemically active colloids [3,4], and quorum sensing interactions in bacterial colonies [5].

Despite a recent surge of interest in non-reciprocal physics a fundamental question remains: do non-reciprocal interactions alter or strengthen the ordered phases of matter driven out of equilibrium? Here, through a combination of experiments and simulations (Fig.1), we show how nonreciprocal forces propel and fission dislocations formed in hydrodynamically driven Wigner crystals.

We explain how dislocation motility results in the continuous reshaping of grain-boundary networks, and how their fission reaction melts driven crystals from their interfaces. Beyond the specifics of hydrodynamics, we argue theoretically that topological defects and nonreciprocal interactions should invariably conspire to deform and ultimately destroy crystals.

Keywords : Non-reciprocity | Colloidal crystal | Hydrodynamic melting

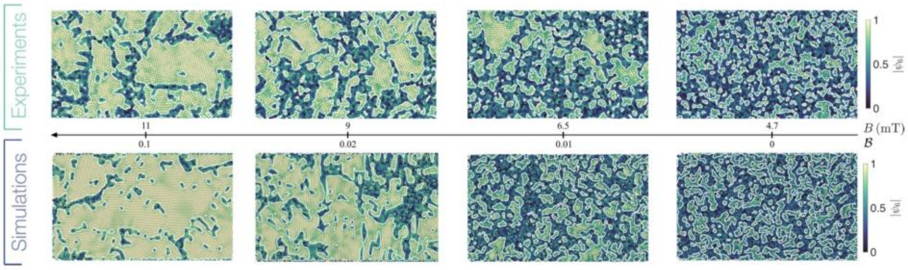

Figure 1: *Variations of the local magnitude of the ψ6 order parameter in our experiments and simulations. Upon decreasing the magnitude of the repulsive magnetic interactions, the system transitions from an ordered hexagonal state to a disordered liquid state. The white lines indicate the position of the grain boundaries.*

Acknowledgments : This work was partly supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement No. [101019141]) (DB). We thank Ephraim Bililign, Yehuda Ganan, Michel Fruchart, and Colin Scheibner for illuminating discussions.

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Matrix viscoelasticity decouples bubble growth and mobility in coarsening foam

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Many soft matter materials evolve through surface tension driven phase separation. During this process the growth of domains can occur via material transfer through the continuous phase. A particular example is foams, which coarsen as gas diffuses between bubbles due to differences in Laplace pressure. In aqueous foams coarsening leads to a characteristic growth of the bubble size, and an accompanying bubble dynamics. However, in many industrial products and processes the continuous phase is not a Newtonian fluid, but a viscoelastic one, such as a paste or a gel. Such foams typically have longer life-times, as the foam ageing processes are slowed down.

We are interested in understanding the role of a viscoelastic continuous phase on foam ageing, and in particular foam coarsening. We study the temporal evolution of foams made from concentrated emulsions. The behaviour of our foams is no longer dominated by capillary effects, as it is impacted by the rheological properties of the emulsion between the bubbles. We show that the yield stress of the continuous phase impacts both the foam dynamics and its structural evolution leading to spatially heterogeneous coarsening [1-3]. The resulting patterns are unlike those observed in aqueous foams. Beyond their importance in the design of foamy materials, the results give a macroscopic vision of phase separation in a viscoelastic medium.

Keywords: foam, emulsion, bubble dynamics

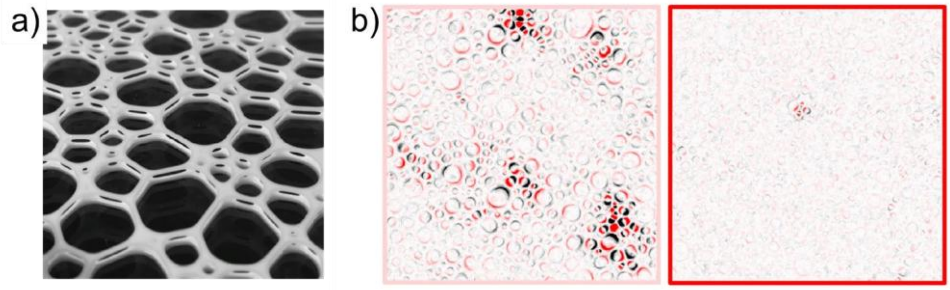

Figure 1. *a) Photograph of a quasi-2D foamed emulsion. b) Activity maps in a foam with rearrangements (left), and in a foam where the continuous phase yield stress hampers rearrangements (right).*

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Stabilizing thin films from rupture using salt

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The production of foam in a salty environment, presents challenges as the ionic strength changes the surfactant interactions, which in turn can result in changes in foam stability. The most drastic destabilization mechanism is coalescence, which occurs as the thin film between bubbles ruptures. We study the impact of salt on film coalescence. A classical experiment consists of pulling a film from a liquid bath (Figure 1 - Left). This experiment has been used to follow film thinning through drainage and evaporation [1]. Recently, a study with a non-ionic surfactant showed that film drainage slows down in the presence of salt because it increases its viscosity [2].

We study the stability of films from solutions of a cationic surfactant, tetradecyltrimethylammonium bromide (TTAB) with and without NaCl. We measure film rupture and film thickness under controlled humidity condition [1]. We have carried out statistics on film rupture and shown that even for films made with solutions containing salt, higher humidity leads to greater stability. [1]. We now show that a film pulled out of a salty bath is more stable (Figure 1 - Right) regardless of ambient humidity. We have measured the film thickness over time at the top of the film. The two-mechanisms responsible for film thinning – evaporation and drainage – are not affected by the presence of salt whatever the atmospheric humidity. Relative humidity only affects evaporation at film thicknesses below 250 nm. Surprisingly, we observed that the primary effect of salt is to stabilize very thin (5 nm) films.

This in-depth study of foam films with salt can provide tools to understand how to stabilize seawater foam, where they can be used for depollution.

Keywords: Foam, seafoam, film, salt, stability

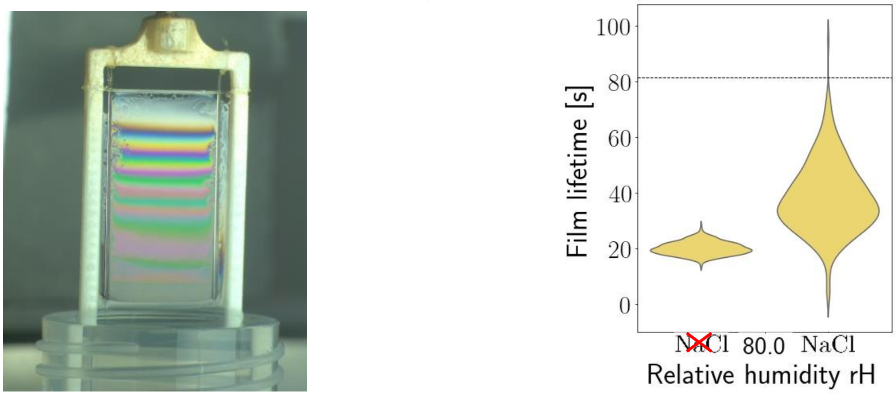

Figure 1. *Left: Photograph of a film before rupture. Right: Distribution of film lifetimes with or without NaCl.*

Acknowledgements: We are very grateful to Laura Wallon for measuring surface tension.

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Mechanisms of polymeric nanoparticle self-assembly in thin films

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Self-assembly at the nanoscale is a key mechanism underlying various biological processes and serves as an effective strategy for designing artificial, multifunctional materials. Understanding the principles of self-assembly is, therefore, critical for both the engineering of functional materials and the elucidation of cellular complexities. In this study, we investigate the self-assembly of polymer-grafted nanoparticles at the air-water interface. Atomic force microscopy (AFM) images reveal intricate bimodal particle patterns, suggesting the emergence of a novel morphology. To explain this phenomenon, we employ a gradient dynamics model for the evaporating of polymer solution thin films on a substrate. By integrating the Flory-Huggins free energy functional, we demonstrate that the competition between dewetting and phase separation instabilities is responsible for the formation of these hierarchical structures in the evaporating polymer films.

Given the general applicability of the model, we propose that it provides a valuable framework for generating morphological phase diagrams that characterize the self-organization of soft polymer-based nanostructures in thin films. Furthermore, nonlinear simulation results reveal a noteworthy correlation between our system and the liquid-liquid phase separation observed in protein condensates.

Keywords: self-assembly, dewetting, phase separation, bimodal patterns

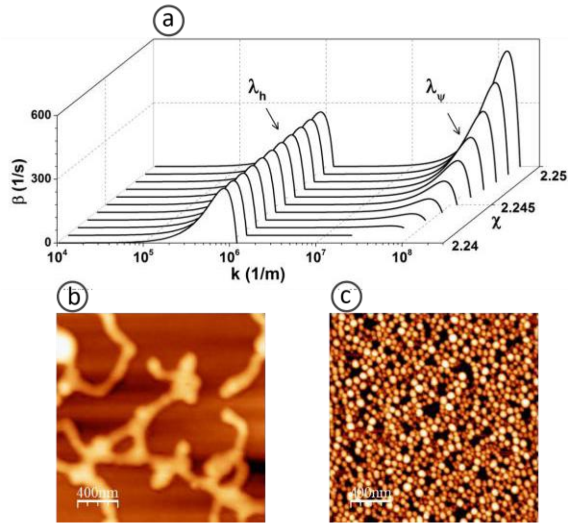

Figure 1. *a) Dispersion curves of polystyrene solution thin film displaying length scales of dewetting and phase separation. b & c) AFM images of bimodal polymeric nanoparticle patterns.*

Synergistic effect of PIP2 and PIP3 on membrane-induced phase separation of integrin complexes

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The assembly of integrin adhesion complexes at the inner leaflet of the plasma membrane regulates cell adhesion to the extracellular matrix. The multivalent protein interactions within the complexes and with the cell membrane display characteristics of membrane-associated biomolecular condensates driven by liquid-liquid phase separation. The composition of lipids and the distribution of the cell membrane are crucial for forming integrin adhesion complexes.

Here, we report that solid-supported lipid membranes supplemented with phosphoinositides induce the phase separation of minimal integrin adhesion condensates composed of integrin $\beta1$ tails, kindlin, talin, paxillin, and FAK at physiological ionic strengths and protein concentrations. We show that PIP$_2$ and PIP$_3$ in the model membrane synergistically regulate the formation of membrane-induced integrin adhesion condensates. The presence of phosphoinositides is key to enriching kindlin and talin on the lipid membrane, which is necessary to further induce the phase separation of paxillin and FAK at the membrane [1].

Our data demonstrate that the preferential bindings of kindlin to PIP$_3$ and talin to PIP$_2$ enhance their recruitment to the membrane, which in turn increases the probability of membrane-associated phase separation. Therefore, lipid membrane surfaces set the local solvent conditions for steering the membrane-localized phase separation. Our results indicate that modulating the intricate balance of membrane composition is a strategy to localize integrin adhesion complexes and optimize their density on lipid membranes [2].

Keywords: Phase separation, Membrane, Lipid, Integrin, Phosphoinositides

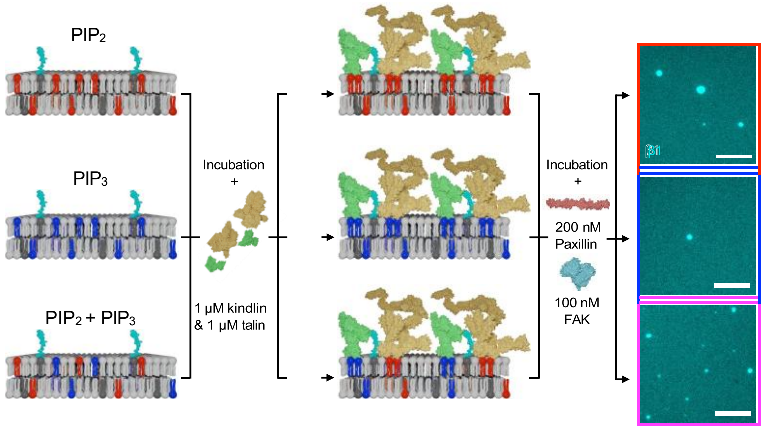

Figure 1. *PIP$_2$/PIP$_3$ membrane synergistically enhances the emergence of $\beta1$ clusters. Scale bars, 10 µm.*

Acknowledgements: We acknowledge financial support by the European Research Council (ERC) under the European 321 Union's Horizon 2020 research and innovation programme (grant agreement no. 810104-PoInt)

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Interaction between marbles in a soap film

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Foam materials are widely used across various industries, from the building industry to the food industry. In liquid foams or bubbles, grains are often embedded within the foam to improve its stability and mechanical characteristics [1]. To understand how particles can stabilize a foam, and to characterize the structural properties of such materials, it is essential to understand the interactions between solid particles in a liquid foam or its fundamental unit: a soap film.

In our experiment, we study the interactions between two millimetric beads placed in a large soap film with a width L~10cm. The beads are initially wet, and thus they are trapped in the film and surrounded by a growing liquid meniscus [2]. When placed one after the other in the film, their trajectory follows intricate orbits (Figure 1): up to 10 full rotations can thus be observed before the beads eventually come into contact. By capturing their motion with a high- speed camera, the interaction force is deduced from the bead dynamic, through successive derivatives of their movement.

We evidence two distinct regimes. At large distances (a few centimeters) the interaction forces arise from the film-scale deformations due to the weight the beads. This interaction is characterized experimentally and modeled theoretically, as a function of the distance between particles and the bead properties (radius, density and age in the film). At short distances (below a few millimeters), the interaction force suddenly increases due to the attraction between the two menisci surrounding the particles. This interaction differs from classical capillary attraction [3] at the surface of a bath due to the contribution of the two interfaces of the soap film.

Keywords: foams, interfaces, bubbles, armored bubbles, particles, capillary attraction.

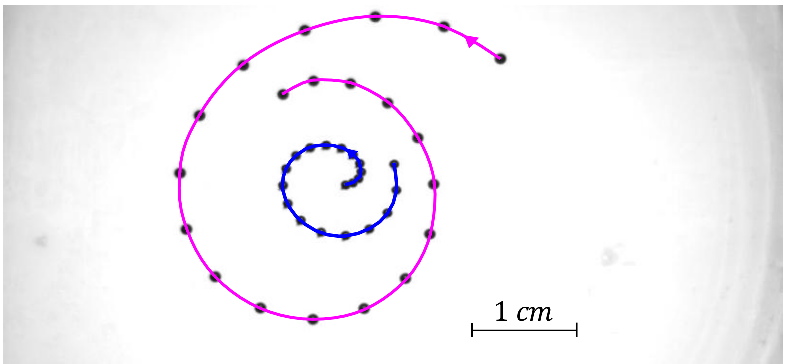

Figure 1 *: Trajectory of two marbles placed in a soap film.*

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Thursday 2nd October 2025

B. Biological and living matter

(Room 3)

Electrochemical regulation of pH-feedback mechanisms of enzyme reactions confined within lipid vesicles

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Biology uses confinement, compartmentalisation and feedback-control of biochemical processes to regulate its complex interplay of parallel functions, leading to highly regulated and robust properties essential for life. We show that surprisingly complex reaction dynamics can be realised within relatively simple biomimetic systems, such as an enzyme reaction confined within a lipid vesicle. We study the reactions of urease, esterase and glucose oxidase enzymes, which all exhibit pH-dependent autocatalytic feedback mechanisms. We demonstrate biomimetic "quorum sensing"-like synchronisation of vesicle behaviour [1] and electrochemical control of proton transport across membranes regulates non-linear reaction dynamics [2]. We also observe systems that give rise to pH pulses and wave-like temporal fluctuations in pH. Reaction-diffusion modelling of these systems uncovers the underlying mechanisms that drive this diversity and complexity of emergent behaviour.

Harnessing these processes will be essential in the design and function of artificial cells and we are already demonstrating application of these systems to develop metabolite-triggered controlled release systems. To this end, we demonstrate a nanoparticle with sustained release of an anticancer drug, Doxorubicin, in response to physiological concentrations of urea. This work advances our understanding of how life might harness systems chemistry within structured soft materials as a strategy to regulate complex function. These insights will also contribute to the engineering of a new generation of biomimetic soft matter for a broad range of technological applications.

Keywords: Vesicles, Membrane Transport, Reaction-Diffusion, Enzymes, Biochemical Feedback

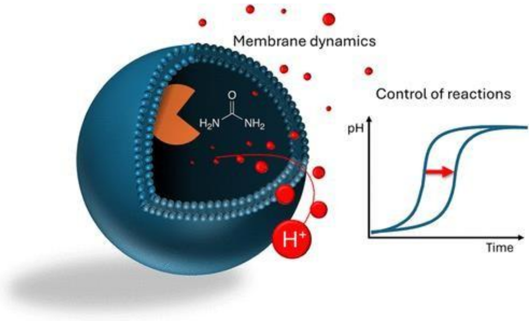

Figure 1. *Electrochemical membrane dynamics regulates enzymatic pH clock reactions confined within vesicles.*

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Elastic Response of Streamer Biofilms to Reversible Flows

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Microorganisms are known for colonizing surfaces and fluid environments by forming organized structures called biofilms [1]. These structures are widespread in natural, technological, and medical settings, often posing a risk of contamination. Understanding the mechanisms of their formation and interactions with the environment is crucial for controlling their spread and growth. A unique case of biofilms are streamers—microbiological filaments formed by cells adhering to one another through an extracellular matrix. They occur in environments where flow prevents full attachment to surfaces.

In our work, we theoretically and computationally investigate a novel method for measuring the bending stiffness of a biofilm. A streamer attached to a cylindrical post is placed in a microfluidic channel and subjected to a uniform external flow [2,3]. Once a steady state is reached, the flow direction is reversed, and the deformation of the streamer is observed. We then use information about the shape and local curvature of the filament as functions of time to infer its elastic properties. In the numerical model, we assume the biofilm is a one-dimensional elastic filament with uniform mechanical properties. We model the streamer as a set of beads connected by springs to capture both its extensibility and bending stiffness. To represent bending, we use a harmonic potential based on the dihedral angles between adjacent beads, along with Lennard-Jones interactions between all beads. To model viscous hydrodynamic interactions, we apply the Rotne-Prager-Yamakawa (RPY) approximation [4].

We focus on the deformation of the filament when it is anchored at one end and exposed to a uniform flow, which is then reversed. The filament flips and undergoes complex deformation, depending on its bending stiffness, length, and the properties of the fluid . The goal of this study is to characterize this transition and how the behaviour depends on system parameters.

Keywords: biofilm, curvature, streamer, elasticity, viscous flow

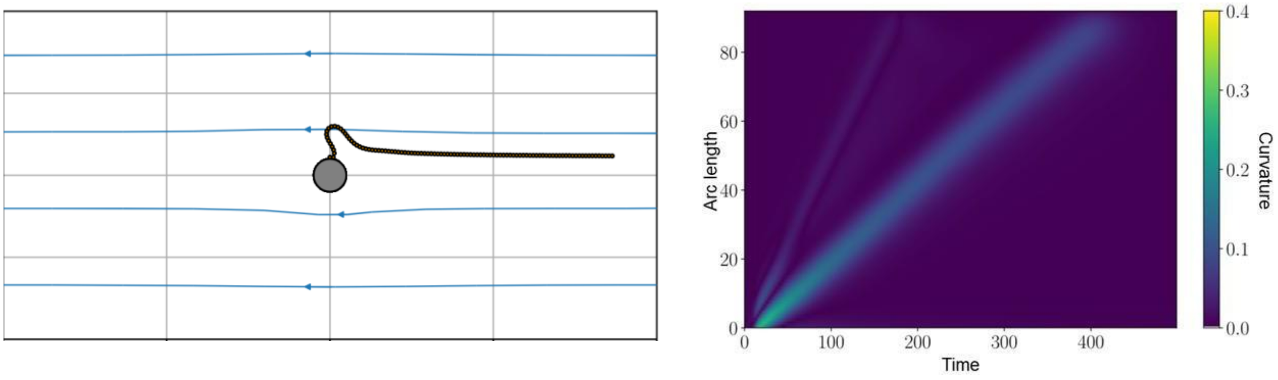

Figure 1. *Example deformation of a fiber for reversed flow (right), kymographs showing how the local curvature changes over time along the entire length of a chain (left).*

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Substrate heterogeneity as a driver of cancer cell dissemination

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While tumor malignancy has been extensively studied under the prism of genetic and epigenetic heterogeneity, tumor cell states also critically depend on reciprocal interactions with the microenvironment [1-2]. This raises the hitherto untested possibility that heterogeneity of the untransformed tumor stroma can actively fuel malignant progression. As biological heterogeneity is inherently difficult to define and control [3], we here chose a highly reductionist bottom-up approach and let tumor cells invade into micro-engineered environments harboring obstacles with precision-controlled geometry. We find that not only the presence of obstacles, but more surprisingly their spatial disorder, causes a drastic shift from collective to single-cell mode of invasion. Combining live-imaging and perturbation experiments with minimal biophysical modeling, we demonstrate that cellular detachments result both from local geometrical constraints and a global temporal integration of the heterogeneity experienced during the invasion process. We show that different types of microenvironments map onto different universality classes of invasion dynamics, which can quantitatively explain our findings. Our findings identify generic physical principles for how the mode of cancer cell invasion depends on environmental heterogeneity, with implications to understand the mechanisms of metastasis *in vivo*.

Keywords: Cancer metastasis, Tumor microenvironment, Active matter, Heterogeneity, Interface dynamics, Numerical simulations

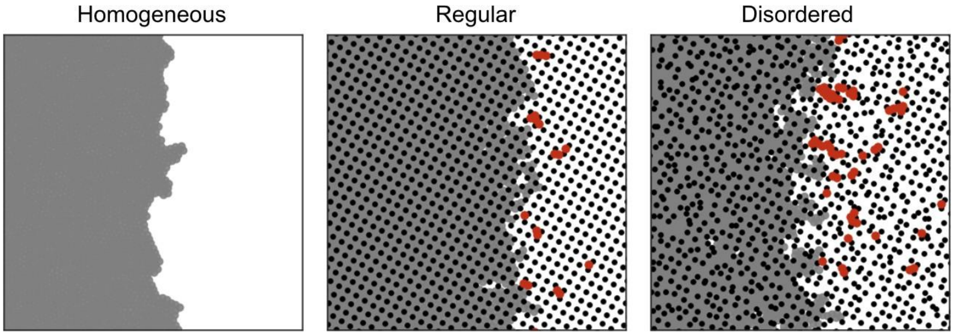

Figure 1. *Snapshots of simulations of cells (grey) migrating in homogeneous environment (left) and invading into regular and disordered array of obstacles (black beads). The detached cells are highlighted in red.*

Acknowledgements: This work has received funding from the Doctoral Programme of the Austrian Academy of Sciences (OeAW): grant agreement 26360.

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Investigating Giant Unilamellar Vesicles Conformation and Membrane Stability: Effect of alpha-amylase mediated starch hydrolysis

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Starch is one of the important micronutrients that humans consume, as it contributes more than 50% of their daily energy consumption [1]. Therefore, extensive research has been conducted to understand the process of starch hydrolysis. Alpha-amylase (AA) is an enzyme that catalyzes the hydrolysis of starch, breaking down its long chains into smaller molecules such as maltose and dextrin. This work elucidates the enzymatic reaction of AA with Giant Unilamellar Vesicles (GUVs) formed in starch solution and the consequent morphological deformations observed due to the reaction. The AA cleaves the starch polymer in the exterior solution of the GUVs, creating bilayer asymmetry [2]. This asymmetry drives the shape deformations and formation of inner buds inside the daughter vesicle which consequently changes the membrane curvature. In this work, we perform video microscopy studies to observe these deformations temporally and substantiate our findings using UV-visible spectrophotometry for different concentrations of AA.
Video microscopy experiments suggest that the conformational changes observed temporally depend primarily on the concentration of AA and the increase in AA concentration accelerates the rate of starch hydrolysis. The initiation, progression, and completion of the conformational changes in these experiments agree with the rate of enzymatic reaction of AA with starch molecules observed in UVvisible spectrophotometry. The stability of the inner buds is determined by the membrane neck curvature and spontaneous curvature of these buds in association with the daughter vesicle [3]. The implications of this work are substantial, offering insights into enzymatic interactions and their effects on membrane dynamics. This knowledge can help us in designing drug delivery systems [4], developing enzyme therapies [5], and many industrial applications [6]. By gaining insights into the AA-starch interactions and their impact on vesicle morphology, this work opens avenues for practical applications in biotechnology, medicine, food science, synthetic biology, and nanotechnology.

Keywords: Alpha-amylase, Starch, membrane neck curvature

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Influence of Crowders and Ligands on the Polymeric Properties of G-Quadruplex Multimers

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G-quadruplexes (G4s) are non-canonical DNA structures formed by guanine-rich oligonucleotides [1]. They are abundant in higher eukaryotic genomes and particularly concentrated in telomeric regions, constituting up to 25% of all DNA G4s [2]. Single-stranded telomeric overhang sequences (ssTELs) can fold into various multimeric G4 configurations with distinct biological roles and interest as potential drug targets [3]. G4 DNA regulates transcription, translation, DNA replication, and RNA localization, but its overall biological roles and those of metabolizing enzymes (e.g., helicases) are not fully understood [4]. Most prominently, G4s have been shown to inhibit telomerase and HIV integrase, which opens the possibility for specific G4-stabilizing compounds to be utilized as anticancer or antiviral medications [5].

Many ligands have been identified to interact with ssTELs to stabilize G4 monomers [6]. Stabilization of ssTELs in cancer cells has been associated with apoptosis [7]. However, ligand effects on the properties of G4 multimers and the mechanisms underlying telomerase inhibition remain unclear. Large-scale, long-timescale computational studies are necessary to address critical gaps in understanding G4 behavior in crowded and non-crowded environments. Elucidating the polymeric properties of G4 multimers is essential to understand relationships between flexibility and biopolymer function.

Using a novel coarse-grained G4 model and molecular dynamics simulations, we study polymeric properties of long telomeric G4 multimers and their modulation by various ligand molecules, both with and without crowders. Our approach is validated against in vitro experiments, demonstrating that long G4 multimers exhibit flexibility akin to polymers in good solvents. In crowded environments, G4 multimers show increased coiling propensity and reduced chain stiffness. Additionally, we demonstrate, in silico, a novel type of ligands we call poly-ligands, that intercalate more effectively into G4 multimers compared to their non-poly counterparts, offering new ways to manipulate the polymeric properties of G4 multimers.

Keywords: G-quadruplex multimers, coarse-grained molecular dynamics, non-canonical DNA, biopolymers.

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Material-fungi interactions

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Engineered living materials (ELMs) are an emerging class of biofabricated materials that integrate living organisms, such as filamentous fungi, into structural matrices to achieve hybrid, sustainable biomaterials. To design effective biohybrid materials, it is essential to elucidate the fundamental interactions between the host materials and fungal growth. Understanding how material properties of the host material such as viscoelasticity, hydrophobicity, anisotropy and nutrient concentration influence fungal growth is crucial for optimizing these materials. This contribution explores fungihost material interactions at the water-air surface, in viscoelastic and lipid host material, in anisotropic scaffolds such as wood hydrogels and in porous host materials as well as host materials of varying nutrient concentrations [1, 2]. Additionally, this contribution explores quantitative methods for assessing mycelial growth, including interfacial shear rheology, compression and tensile testing, and fungal mycelium biomass as a proxy for growth analysis. As a result, we can show that anisotropic wood hydrogels acting as growth template and by increasing the concentration of carbon sources in the host material enhances mycelial network density, leading to improved properties such as stiffness in a mycelium biocomposite [3, 4]. Additionally, quantifying fungal biomass using fungalspecific ergosterol enables differentiation of biomass accumulation across various growth directions, providing a novel approach to studying three-dimensional mycelial growth in solid-state fermentation [5]. This work provides new insights into designing host material for optimal fungal growth and morphology, along with effective methods for quantification. It demonstrates that fungal growth in templated substrates provides a framework to design biofabricated materials

Keywords: fungi, mycelium, engineered living materials, host material, ergosterol

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Cell shape through the eyes of geometry processing

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Biological membranes display a variety of different shapes depending on their function and their environment. Simulating different environments using the common molecular dynamics or Monte Carlo techniques can easily become computationally expensive. In this project I am developing a reliable and fast membrane simulator using triangle meshes and tools from computer graphics. Using tools from discrete differential geometry we are able to replicate known results for spherical particles uptake and tube pulling. I next explore the use of this geometry processing techniques to study complex cell shapes involved in different ecological environments such as the interaction of the cell membrane with different agents mimicking food sources and predators. Our research aims to make research on biological membranes in long timescales more accessible by mixing knowledge from computer graphics with biophysics.

Keywords: Membranes, Simulation, Geometry processing

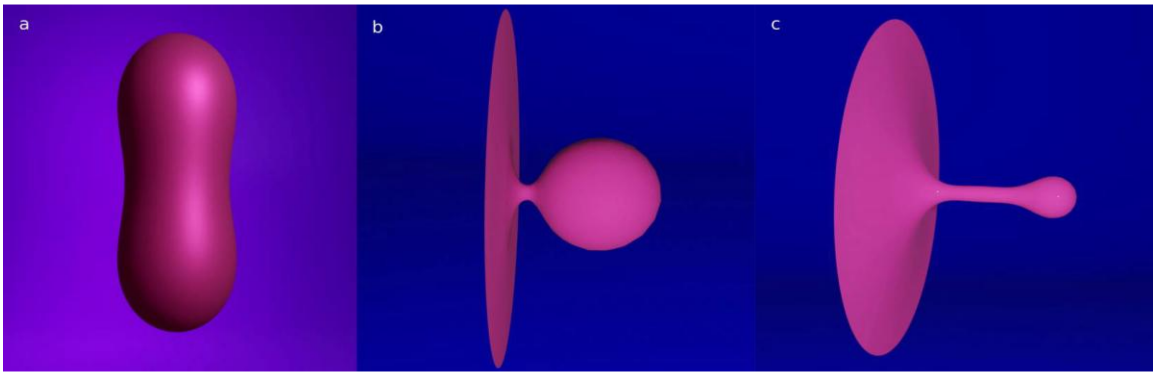

Figure 1. *a) Prolate shape obtained by minimizing the bending energy with fixed volume and area. b) Complete wrapping of a spherical particle by a flat membrane c) Tube pulling of a planar membrane using a spherical particle at the point of pulling.*

Effect of 2D confinement and substrate properties on bacterial self-organization at surfaces

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Surface-attached bacterial colonies are a well-known example of living active matter, exhibiting collective behaviors that play an important role in the spread of microbial infections. In particular, nematic alignment, collective motion driven, and a transition from 2D monolayers to 3D biofilms result in recalcitrant and dangerous colonies. While the underlying mechanics of these behaviors have been described in model systems, many open questions remain about how microbial self-organization adapts to the variety of different environments bacteria encounter in natural and clinical settings.

Here, using novel imaging and computational analysis techniques [1], the effects of physical surface properties and dimensional confinement on the collective behaviors of pathogenic bacteria are described. Biofilm-forming bacteria are grown in microfluidic flow chambers on different substrates, either open to the surrounding fluid or confined to a single monolayer between two surfaces. Orientational ordering in the colony, cell morphologies, trajectories, and growth rates are measured using single-cell segmentation and tracking. The 2D confinement of the bacteria as well as the composition of the substrate are shown to significantly alter their self-organization, their attachment to the substrate, and their single-cell morphology and swimming behavior. Under confinement, distinct layer formation driven by topological defects is observed, followed by collective verticalization and the formation of densely packed crystalline structures exhibiting long-range order. Surprisingly, fixed attachment of cells to the substrate is reduced by 2D confinement, while cell motility is temporarily enhanced and the mean cell aspect ratio is reduced.

These results demonstrate the remarkable breadth of collective behaviors exhibited by bacteria in different environments, which must be considered to better understand bacterial colonization of surfaces. Changes to cell attachment and self-organization that ultimately lead to biofilm formation have important implications for the progression of bacterial infections in physiologically relevant settings.

Keywords: Biophysics, active matter, bacterial self-organization, biofilms

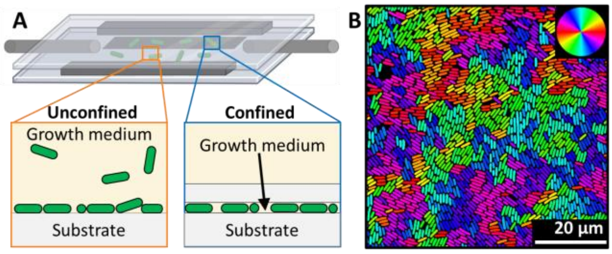

Figure 1. *(A) Schematic of microfluidic device. (B) Confined bacterial monolayer after single-cell segmentation, with each cell colored by its orientation.*

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Unsteady flow effects in cilia-mediated transport

Rafał Błaszkiewicz [1], *Margot Young* [2], *Albane Théry*[2], *Talia Becker Calazans*[2], *Arnold J.T.M.Mathijssen*[2] *and Maciej Lisicki* [1]

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Cilia play a crucial role in biological systems, facilitating locomotion in unicellular eukaryotes, nutrient uptake in marine organisms, and fluid transport in human tissues. While ciliary flows are often modeled as steady, the role of unsteady, inertial effects in low Reynolds number environments remains underexplored. Ciliary beating generates unsteady Stokes flows when the actuation timescale is comparable to or shorter than the viscous diffusion timescale [1]. To investigate these dynamics, we analyze a model governed by time-dependent, linear Stokes equations, which we solve using Green's functions with analytically defined memory kernels [2].

We examine flows induced by time-varying forces that mimic individual and collective ciliary motion, using the "Pufflet"—a point-like hydrodynamic singularity—as a fundamental building block. Combining theoretical analysis, simulations, and experiments (Fig.1.), we explore fluid transport under rapid actuation. We show that unsteady effects enhance fluid mixing by breaking time-reversal symmetry. Vorticity diffusion in this regime generates complex trajectories of advected particles, significantly altering transport efficiency. When multiple actuation sites are introduced, we identify emergent transport patterns that can be optimized through spatial and temporal tuning of the forcing.

Our findings reveal fundamental differences between steady and unsteady Stokes flows, shedding light on microscale transport mechanisms. Understanding these effects may inform the design of bio-inspired fluid systems and optimized microscale mixing strategies.

Keywords: Unsteady Stokes flow, Low Reynolds number, Cilia, Transport in viscous flows

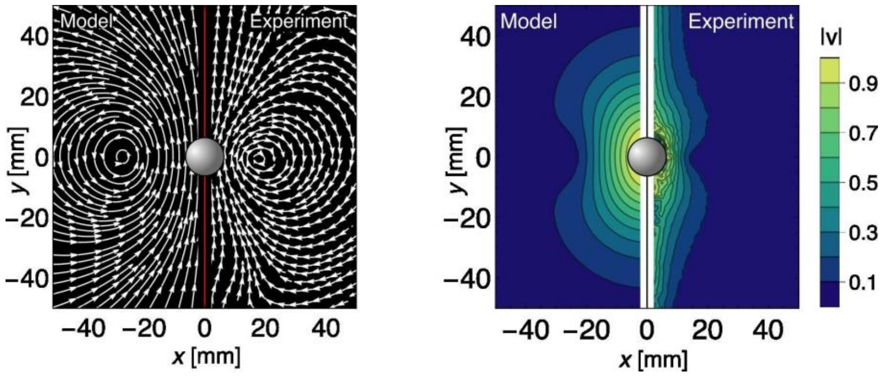

Figure 1. *Flow field comparison between model and experiment for streamlines and magnitudes.*

Acknowledgements: National Science Centre of Poland grant no. 2023/50/ST3/00465 to ML.

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DNA-Programmable Emulsions

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How collections of building blocks efficiently organize into structures with high fidelity is a central question in both biology and materials science. Here we show that linear chains of DNA-functionalized colloidal droplets (ABAB...) successfully fold into unique 2d foldamer geometries [1], which in turn bind to form nets that can efficiently wrap into icosahedral shells in 3d using optimized temperature protocols. These colloidal capsids can then be opened and closed using enzymatic dynamics that write, cut, and modify the DNA interactions to assemble, disassemble, and reconfigure these structures. Finding such designable self-assembling systems presents a promising route to functional materials that serve a purpose, such as targeted drug delibera and reactive surfaces.

Keywords: droplets, emulsions, colloidal machines

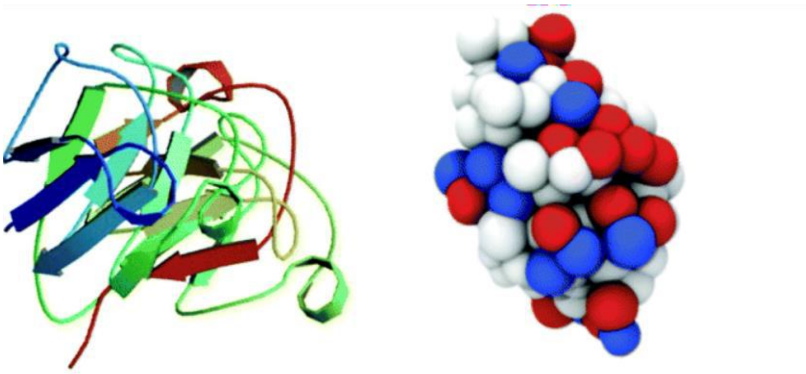

Figure 1: A biological protein modeled in a way that each amino acid is represented by a droplet carrying a different flavor of DNA.

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A new perspective on lung surfactant inactivation and possible Treatments

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Lung surfactants, a mixture of lipids and proteins, play a vital role in increasing pulmonary compliance and reducing the energy required for breathing [1]. During inflammation, the bulk becomes enriched with lysolipids and serum proteins, leading to surfactant inactivation [2,3]. Previously, it was suggested that these inflammation components adsorb faster at the air-liquid interface, creating an electrostatic barrier that hinders lung surfactant adsorption [2]. However, our results from dynamic thin film balance experiments reveal that the disjoining pressure of a lung surfactant thin film remains unchanged in the presence of inflammation products, hinting that competitive adsorption is not responsible for surfactant inactivation. On the other hand, the dynamic evolution of the thin surfactant layer is significantly altered, hinting to a different mechanical behavior. By integrating these results with radial trough measurements and cryogenic transmission electron microscopy (cryoTEM), we provide new insights into how mechanical response alterations drive surfactant inactivation. These findings emphasize the necessity of considering structured interfaces in therapeutic strategies to restore surfactant function under inflammatory conditions.

Keywords: Lung surfactants, dilatational rheology, interfacial properties

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Thursday 2nd October 2025

BF. Biomedical & Food applications

(Room 3)

Biopolymers based ROS- and GSH- responsive nanocarriers for the delivery of therapeutics

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Stimuli responsive nanocarriers (NCs) have continuously gained attention for drug delivery applications. Particularly, NCs based on responsive polymers have gained attention owing to their ability to undergo change in structural conformation/composition under the influence of various physical, chemical and biological stimuli. In complex biological microenvironments, responsive nanocarriers responding to endogenous triggers are of significant interest as payload can be released rapidly and selectively by taking advantage of a unique biochemical environment (e.g., difference between tumor and normal tissues). As redox imbalance (excess reactive oxygen species (ROS) and glutathione (GSH) production) is characteristic of many disease conditions (e.g., tumor, inflammation), NCs designed for cargo release at the target sites that exhibits high ROS/GSH levels has evoked enormous interest.

As dextran and hyaluronic acid (HA) are widely used biopolymers in the development of various drug delivery platforms, in this contribution, our recent work on the ROS and GSH responsive biopolymers based NCs and their potential in cancer therapy will be presented[1,2]. In case of dextran based NCs, dextran conjugated with ROS responsive moieties is synthesized and hydrophilic payload containing NCs were formulated using interfacial polymerization employing the miniemulsion technique[1]. While in case of HA based responsive NCs, a small bifunctional GSH responsive linker molecule is mixed together with HA in the NC formulation[2]. NCs were successfully synthesized varying several reaction parameters and subsequently characterized. The encapsulation efficiencies of the various hydrophilic payloads in the NCs were between 80-95%. The release kinetics systematically studied under respective ROS and GSH conditions showed a clear stimulus responsive release trend. Additionally, release was studied using enzymes that can degrade the biopolymers. Biocompatibility and cellular uptake experiments were also carried out. The promising results highlight the huge potential of biopolymer based responsive NCs to deliver hydrophilic therapeutics in complex biological milieu as in tumor.

Keywords: ROS-responsive, GSH-responsive, nanocarriers, biopolymers, drug delivery

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3D bioprinted complex constructs for enhanced osteogenic and anti-osteoclastogenic potential

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Bone remodeling is a dynamic process balancing osteoblast-mediated bone formation and osteoclast-driven resorption, crucial for skeletal integrity. Mechanical cues from the microenvironment regulate this balance, which can be disrupted by aging, trauma, or diseases like osteoporosis, leading to impaired regeneration.

To address these challenges, a novel bioink was developed using two natural polysaccharides, alginate (ALG) for stability and ionic crosslinking, and methylcellulose (MC) for enhanced mechanical properties, printability, and thermosensitivity. To improve biological functionality, an elastin-like recombinamer (ELR) functionalized with an RGD sequence was incorporated, mimicking the extracellular matrix (ECM) and promoting cell adhesion [1]. Additionally, 2 wt% of 50% strontium-substituted nanohydroxyapatite (Sr-nHA) was integrated to support bone remodeling, as strontium inhibits osteoclastogenesis, while hydroxyapatite promotes osteogenesis [2].

Physicochemical and biological characterization was conducted on three bioink formulations, 3 wt% ALG/2 wt% MC, 3 wt% ALG/3 wt% MC, and their ELR-functionalized variants with 1 wt% ELR. FTIR analysis confirmed successful component integration.

Swelling ratios ranged from 40–50%, and degradation studies showed favorable mass loss over 21 days. Improved mechanical properties in MC-containing formulations, with Young's modulus reaching 250 kPa for 3 wt% ALG/3 wt% MC, compared to 120 kPa for the ALG control. Printability assessments showed superior accuracy of 80% for 3 wt% ALG/3 wt% MC, while the control bioink exhibited the lowest accuracy of 20%. Cytotoxicity assays confirmed high biocompatibility, with ELR-functionalized bioinks showing improved cell viability.

The developed bioink integrates structural stability, enhanced printability, and bioactivity. The incorporation of Sr-nHA provides an additional osteo-regenerative capacity, potentially guiding the osteoblast-osteoclast balance. Ongoing studies assess the bioinks' ability to regulate osteoclastogenesis and osteogenesis with the incorporation of bone marrow-derived mesenchymal stem cells (BM-MSCs) and peripheral blood mononuclear cells (PBMCs) into the constructs. Their differentiation capacity will be assessed under dynamic conditions that mimic physiological mechanical loading, offering insights into the development of biomaterials tailored for personalized bone regeneration strategies.

Keywords: Bone tissue engineering, osteogenesis, osteoclastogenesis, 3D printing, composite scaffold

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Deciphering the organelle-targeting specificity of inducible amphipathic helices through a recombinant protein platform

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Many cytosolic proteins critical to membrane trafficking and function contain an unstructured domain that can bind to specific membranes, with a transition into an amphipathic helix induced upon membrane association. These inducible amphipathic helices often play a critical role in organelle recognition and subsequent function by these cytosolic proteins, but the tools and techniques used to characterize affinity towards specific membranes are low-throughput and highly dependent on the solubility of the inducible amphipathic helix.

Here, we introduce a modular recombinant protein platform for rapidly measuring the binding affinity of inducible amphipathic helices towards a variety of membrane compositions and curvatures using high-throughput fluorescence anisotropy measurements (Figure 1). Inducible amphipathic helices are solubilized with a fluorescently tagged small ubiquitin-like modifier (SUMO) protein and binding to membranes quantified by leveraging the unexpected decrease in fluorescence anisotropy upon binding, a phenomena previously observed but not well understood. By using fluorescence anisotropy decay measurements and solution NMR experiments, we deduce that this phenomenon likely occurs due to the local increase in fluorophore motion upon binding to the membrane.

We apply this approach to representative inducible amphipathic helices to determine the peptide code by which they specifically target organelles. By systematically varying membrane parameters, we identify key physiochemical features that drive selective binding of inducible amphipathic helices with the goal of enabling predictive models for how sequence dictates organelle targeting within cells.

Keywords: Inducible amphipathic helix, intrinsic disorder, protein-membrane interactions, high-throughput screening

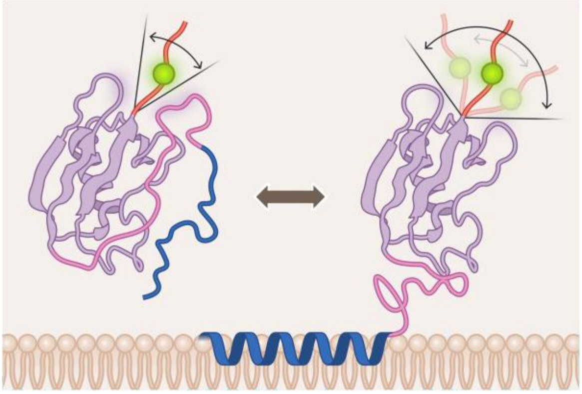

Figure 1. *A model of our recombinant protein platform, with the inducible amphipathic helix (blue) binding upon recognition of its cognate membrane. High-throughput reporting occurs via a local increase in fluorophore mobility.*

Understanding Fundamental Molecular Mechanisms of Lipid Membranes and Developing Design Principles for Biomimetic Membranes

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Direct angstrom-level, nano-Newton force measurements with the surface force balance (SFB) have revealed that phospholipids, in the form of single-component lipid bilayers, are remarkably effective biolubricants, with friction coefficients comparable to those of synovial joints such as hips and knees. However, synovial joints contain over a hundred lipid species. This proliferation of lipids raises a central question: is it natural redundancy, or does it contribute synergistically to optimize lubrication at cartilage surfaces?

Existing SFB experiments on a limited number of mixed-lipid membranes have demonstrated that certain combinations can exhibit superior lubrication properties, yet the underlying physical principles remain unclear. To address this, we investigate the roles in the mixed-lipid membranes of the most common synovial lipids, and relate their presence to the synergistic behavior observed at the holistic level, particularly in dynamic membrane processes such as hydration lubrication and hemifusion. This research integrates molecular dynamics simulations, artificial intelligence, and AI-guided AFM experiments, enabling high-throughput exploration of the vast parameter space of mixed-lipid membranes. We also use the SFB—with its unique sensitivity and resolution in measuring membrane interactions —to validate and refine our conclusions.

As our understanding of these biophysical processes deepens, we can better interpret the design principles shaped by evolution and assess the extent of possible redundancy. Ultimately, these bio-inspired insights will guide the development of artificial, biocompatible lipid membranes with a spectrum of properties depending on their composition. These range from better lubrication treatments at one end, as for widespread joint-related diseases such as osteoarthritis, to better drug-delivery by lipid-based nanocarrier vesicles (liposomes or lipid nanoparticles) at the other, through more facile vesicle-membrane/cell fusion processes.

Keywords: hydration lubrication, lipid membranes, synovial fluid

Quantification of exogenous mRNA translation and degradation at single-cell and population level

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The importance of mRNA technology has become undeniable, particularly following its success in COVID-19 vaccines. While its potential in cancer immunotherapies is equally promising, it remains less widely recognized. Current research focuses on improving mRNA stability, translational efficiency, and delivery methods, such as lipid nanoparticles. However, a significant gap exists in the quantitative characterization of mRNA's physicochemical properties, as most available methods remain qualitative.

In this study, we present a quantitative approach to determining mRNA translation and degradation rate constants at the single-cell level. Using confocal microscopy with time-correlated single photon counting (TCSPC), fluorescence correlation spectroscopy (FCS), and fluorescence microscopy imaging combined with object recognition and tracking, we analyze mRNA constructs encoding fluorescent proteins (eGFP, mKate2). These constructs are introduced into living cells via microinjections. In the case of mRNA translation, we demonstrate up to 12 hours of fluorescence-based single-cell analysis to quantify real-time protein production kinetics. For mRNA degradation, fluorescence images are recorded over several days at approximately one-hour intervals. Image analysis allows us to track fluorescence intensity over time, either across the entire population or at the single-cell level when using cell-tracking software.

We obtain numerical values for mRNA translation and degradation rate constants byfitting the resulting time-intensity or time-concentration curves to kinetic models. Our models account for three key processes: mRNA translation (protein production), mRNA degradation, and protein degradation, all treated as pseudo-first-order reactions. We assume a gamma distribution of rate constants across the observed cells when analyzing population-averagedsignals. This methodology provides a quantitative framework for studying mRNA stability and degradation dynamics, addressing a crucial need in the field.

Keywords: mRNA degradation, Fluorescence microscopy, Kinetic modeling, Single-cell level

Acknowledgments: This work was co-financed by the Polish Science Fund, Virtual Research Institute, within the grant WIB-1/2020-0n; WIB_HERO

Cationic Degradable Polyesters with pH- and Salt-Responsive Behavior and Tunable UCST in Aqueous Media

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Thermo-responsive polymers are promising "smart" materials that have been proposed for diverse applications.[1] While lower critical solution temperature (LCST) polymers are well-studied, their upper critical solution temperature (UCST) analogues in water remain rather unexplored. The majority of the UCST systems rely on non-degradable polymers, which raise environmental concerns and limit their biological applications, whereas degradable UCST polymers are scarce.[2] Polycations, which hold potential for use in gene/drug delivery, tissue engineering, and antimicrobial applications, can exhibit UCST in the presence of specific anions. [3-5]
Herein, we present the synthesis of degradable polycations based on main chain polyesters that exhibit pH- and salt-responsive properties, as well as an UCST behavior in water at specific salt concentrations. Featuring quaternary ammonium salt side groups paired with Cl^- or BF_4^- anions, these polyesters are water-soluble under physiological conditions and exhibit tunable UCST-type transitions upon salt addition. The polymers were synthesized via a polycondensation reaction followed by thiol-ene click chemistry and exhibit tunable cloud points (8-91°C) across a broad pH range (pH 4.0-7.4), controlled by adjusting the polymer concentration, salt-to-cationic repeat monomer unit ratio, and counter-anion type. Moreover, the main chain polyesters demonstrated significant hydrolytic degradation under physiological conditions. These "smart", degradable materials present significant potential for various applications owing to their adjustable and environmentally benign properties.

Keywords: degradable polymers, UCST, polyesters, polycations

Acknowledgements: Acknowledgments
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Thursday 2nd October 2025

Active matter/ Experimental & Computational Methods (including AI)

(Room 4)

Active particles in tunable crowded environments

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Active particles affect their environment as much as the environment affects their active motion. In this work, we present a versatile experimental model system where both can be simultaneously adjusted *in situ* using a single control knob [1]: the strength E of an applied AC electric field. The environment consists in a two-dimensional bath of colloidal silica particles that are polarized and interact via long-range dipole-dipole pair potentials; as we increase the electric field, the colloidal background freezes and becomes more solid (Fig. 1(a) to Fig. 1(b)). The active particles are Janus spheres that self-propel through an induced-charge electrophoresis mechanism at velocities proportional to E^2 [2].

The feedback between environment and self-propulsion significantly alter the active Brownian motion of the Janus spheres. As we observe our system under a microscope, the Janus particles plough their way through the crowd of repulsive spheres, shovelling them aside. However, with stiffer environments and faster speed, they reorient much faster (Fig. 1(a) to Fig. 1(b)). At the largest fields, they even start circling around and undergo a helical motion, as if they were chiral. The underlying mechanism is resolved by numerical simulations: an initial strong direction fluctuation compresses the colloidal matrix asymmetrically and thus leads to an asymmetric reaction favouring sustained turns to the same side. Our model system provides a minimal microscopic description of memory effects reported for active particles in viscoelastic fluids [3].

Keywords: active matter, colloids, Janus particles, viscoelasticity.

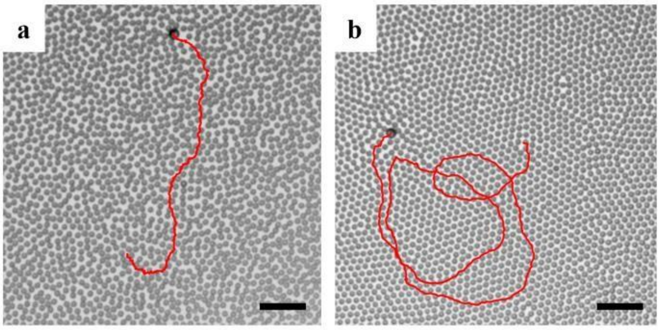

Figure 1. *Snapshots of Janus particles cruising in colloidal monolayers of Brownian microspheres under applied electric fields (a) E = 42 V/mm and (b) E = 108 V/mm. The scale bar corresponds to 20 µm in both microscopy images.*

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Critical role of the motor density and distribution on polar active polymers

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Active polymers, driven by biological motors, play a key role in cellular functions. Cytoskeletal filaments like actin and microtubules move under forces generated by motors such as kinesin and myosin [1]. In this process, these molecular machines consume chemical energy and exert mechanical forces on the polymer. In this work, we explore the conformational changes in polymers induced by such polar active forces. Unlike models that assume uniform activity [2], we study polar filaments with active pockets, closely resembling real bio-polymers. Our simulations reveal that motor density and its spatial arrangement play a vital role in determining polymer conformations, leading to a loss of self-similarity. These structural changes significantly impact self-propulsion velocity and relaxation time [3].

Keywords: Polar filaments, globule structures, stretched structures, motor density.

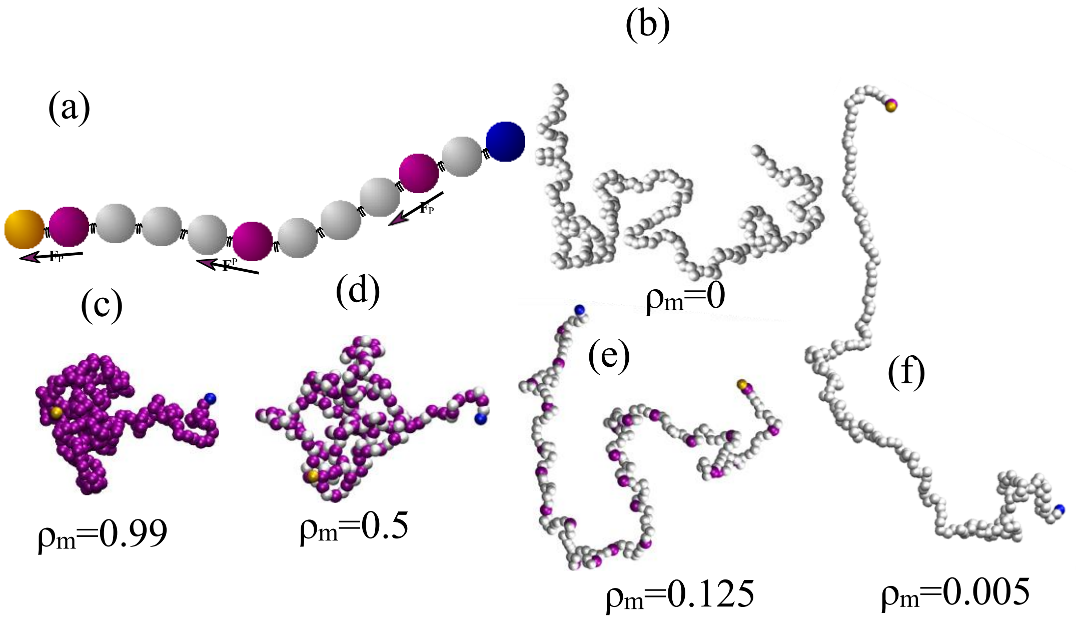

Figure 1. *Polar polymer structure and typical configurations. (a) Polymer sketch with head bead in yellow, motor beads in purple, tail bead in blue, and linker beads in white. The arrows indicate the direction of the polar active force. Snapshot for the passive polymer is depicted for reference in (b), while snapshots from (c) to (f) illustrate globule to stretch conformations with decreasing motor densities (ρ_m) for the chain length N=200 at Pe=17.*

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Active Colloids in 3d: Travelling Strings, Shaking Labyrinth and Novel Crystal Excitations

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Understanding of collective behaviour in active systems is massively enhanced by minimal models which nevertheless capture its essence. Active colloids provide an important class of model systems, exhibiting the exotic collective behaviour of animal groups, such as milling in fish [1], yet in a setting where the interactions which underly the macroscopic phenomena may be precisely controlled. Active colloids furthermore present opportunities for smart actuated materials and microrobots.

Until now, experiments with active colloids have been largely limited to (quasi) 2d systems. We may reasonably expect that moving to three dimensions will bring new phenomena. Here we introduce a 3d active colloidal system of Janus particles comprised of a dielectric where one hemisphere is coated with metal which is itself coated with the insulator. Under an AC electric field, this system is active in the plane perpendicular to the field and acquires a dipolar interaction parallel to the field [2].

Our 3d active colloids exhibit a complex and intriguing set of unexpected behaviour: travelling strings of particles, which can be described as active polymers [2] along with sheet-like and labyrinthine assemblies which fluctuate in a manner reminiscent of biological membranes. Surprisingly, the active sheets and labyrinth break symmetry in a direction perpendicular to the applied field. Finally, and perhaps most remarkably for an overdamped system, the 3d colloidal crystal that forms features long-wavelength fluctuations reminiscent of phonons.

Keywords: Active Colloids, Active Matter, Active Crystal

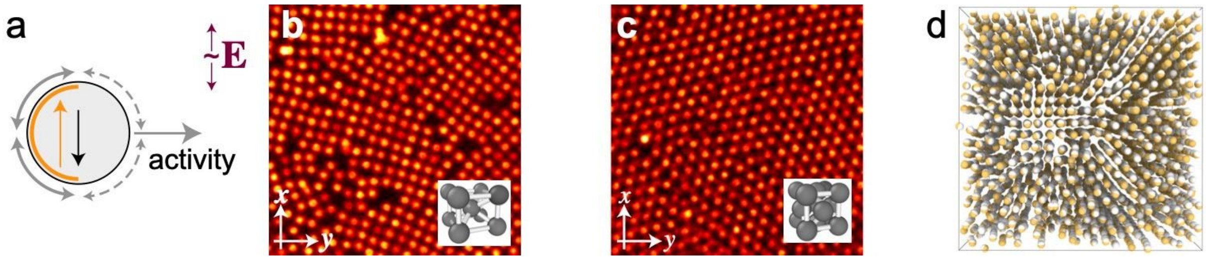

Figure 1. *Overview of crystallisation in the 3d induced-charge electrophoresis system. (a) Schematic of an induced charge electrophoresis particle. The movement of ions around the particle due to the AC field is indicated by the dashed grey lines. (b) Confocal microscopy image of body centered tetragonal crystal in the xy plane. (c) Confocal microscopy image of HCP crystal in the xy plane. (d) Rendering of 3d coordinate data for a body-centred tetragonal (BCT) crystal.*

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Autophoresis near permeable surfaces

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The dynamics of self-propelled colloidal particles are strongly influenced by their environment through hydrodynamic and, in many cases, chemical interactions. We develop a theoretical framework to describe the motion of confined active particles by combining the Lorentz reciprocal theorem with a Galerkin discretisation of surface fields, yielding an equation of motion that efficiently captures self-propulsion without requiring an explicit solution for the bulk fluid flow. Applying this framework, we identify and characterise the long-time behaviours of a Janus particle near various interfaces – rigid, permeable, and fluid-fluid – revealing distinct motility regimes, including surface-bound skating, stable hovering, and chemo-hydrodynamic reflection. Our results demonstrate how the solute permeability and the viscosity contrast of the surface influence a particle's dynamics, providing valuable insights relevant to experimental design and the controlled guidance of autophoretic particle systems. The computational efficiency of our method makes it particularly well-suited for systematic parameter sweeps and many-body simulations, enabling the identification and analysis of collective behaviours in confined autophoretic particle systems.

Keywords: active matter, Janus particles, colloids, phoresis, low-Reynolds-number flows, collective dynamics

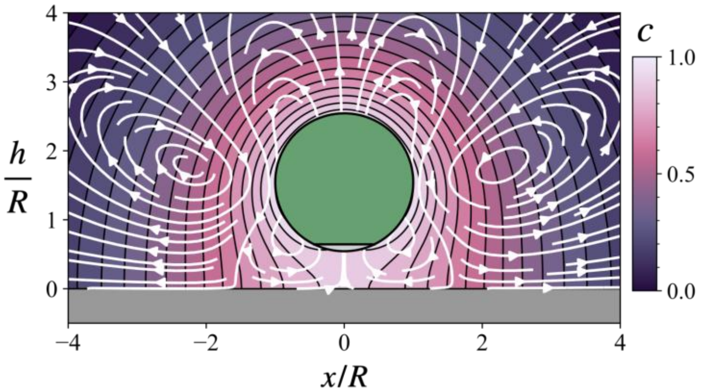

Figure 1. Hovering above a permeable surface. *A neutrally buoyant Janus particle with a large catalytic cap (green) in a stable hovering state at height h above a chemically permeable wall (grey). In this state, the particle acts as a stationary micro-pump, advecting the surrounding fluid, as indicated by the streamlines (white arrows). The normalised concentration field c generated by the particle is represented by the overlaid colour map.*

Active colloidal assembly

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Active assembly and dis-assembly are fundamental processes, central to any living organism from molecular to (eco)system level. Examples include biopolymers such as actin filaments, whose structure is regulated by assembly on one side and disassembly on the other, or molecular selection, which is often regulated by kinetic bias. In these processes, active assembly typically happens much closer to equilibrium than disassembly; the reason for this imbalance remains obscure.

To reveal active assembly principles, we combine recent most elementary model systems of patchy and active particles: colloidal patchy particles with directional interactions allow forming analogues of molecules [1,2] at optically observable length scales. Combining these building blocks with active particles that bind to the assembling structures and move autonomously by chemical gradients or applied fields, we obtain unprecedented insight into active assembly. We observe that at low activity, the assembly becomes strongly enhanced, and the assembly time shortens dramatically. Microscopic imaging shows that this is due to transport of particle clusters by the active particles, breaking the diffusion limit. Beyond an activity threshold, however, the trend reverses: activation causes structural breakup and fragmentation, leading to active disassembly far out of equilibrium. We describe both processes, enhancement and breakup, by rate equations involving the measured activity-dependent association and dissociation rates, and use accompanying simulations to model the resulting nonequilibrium steady states. Furthermore, we show that application of active particles to patchy particle mixtures forming equilibrium networks [3], allows us to actively tune the system towards percolation and de-percolation with activity magnitude, while fundamentally changing the mechanical properties of the structure.

These results provide insight into the regulatory mechanisms central in biology, yet afforded by the simple fundamental effect of activity, regulating structures and adapting them quickly. These principles also offer concepts for a wide range of new adaptive synthetic materials.

Keywords: active matter, colloidal assembly, patchy particles, colloidal swimmers

Acknowledgements: We acknowledge funding (Grant No. 680.91.124) from the Netherlands Organization for Scientific Research (NWO).

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Kinetics of phase transition in nonreciprocal mixtures of passive and chemophoretically active particles

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We study phase separation kinetics in two-dimensional binary mixtures of active and passive colloids [1-2]. An active particle acts as a source (S) of the chemical gradient to induce phoretic motion among the passive (P) particles (Fig. 1). Mediated by this effective long-range interaction, the suspension undergoes a phase separation resembling a vapor-liquid-like phase transition. Via simulations, incorporating Langevin dynamics, we construct the related steady-state phase diagram. We exploit this knowledge to study the structure and growth associated with kinetics following sudden quenches of homogeneous systems into the miscibility gap, for far-from-critical and near-critical densities. An advanced finite-size scaling technique is employed to calculate the related growth exponents accurately in the thermodynamically large system size limit, using data from systems of several different finite sizes, for each of the cases. The growth data are described well by a recently constructed analytical function [3], irrespective of system size and particle density. Our results reveal a significant enhancement in the rate of domain growth with increasing phoretic strength—an effect absent in equilibrium systems. For the off-critical case, I will also discuss the possible underlying growth mechanisms within an appropriate theoretical framework.

Keywords: Chemophoresis, non-reciprocal interactions, self-assembly, phase transitions

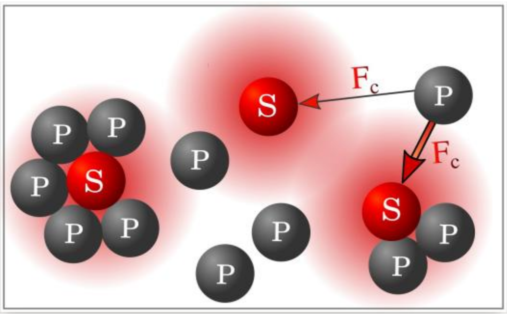

Figure 1. *Schematic illustration of a mixture of source (S, red) and phoretic (P, black) colloids. The S particles act as the reaction centers that produce a radially outward chemical gradient. Fc represents the corresponding phoretic interaction between S and P.*

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Designing run and tumble dynamics of active lipid vesicles

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The creation of bioinspired microswimmers with adaptive motility presents significant potential to de- sign advanced synthetic cells and biomimetic systems. Colloidal active swimmers are broadly used as model systems to design microscopic swimmers, yet their rigid and solid architecture limits their adaptability and functionality. A promising alternative is using soft compartments such as giant unilamellar vesicles (GUVs) [1] as biological scaffolds for the design of cell-mimetic motile architectures.
Here, we fabricate phase-separated Janus lipid vesicles [2], harnessing the fluidity of lipid membranes to achieve reconfigurable motion. Under external electric fields, these asymmetric compartments self-propelled, and exhibit transient *run-and-tumble-like* dynamics due to the membrane fluidity interacting with the electric field [3]. Moreover, by adjusting the lipid composition and using temperature as an external trigger, we modulate membrane fluidity and phase separation. Thus, we tune in-situ the frequency of tumble events by controlling the mixing of both phases [4]. We study the spatial-dependent motion under stable temperature gradients leading to interesting dynamical patterns. Our findings demonstrate the potential of synthetic cell membranes as architectures to replicate the intricate motility reminiscent of cells, providing an important step toward creating next generation microswimmers relying on the inherent reconfigurable membrane properties.

Keywords: active matter, soft microswimmers, Janus vesicles, phase-separation

Acknowledgements: V. W. and L. A. are thankful to Prof. M. Angelova, and Prof. H. Kellay for fruitful discussions. L.A. and V.W. acknowledge IdEx Bordeaux (France) for financial support. J.-C Baret acknowledges the support of the `Fondation Simone et Cino Del Duca' and of the Univ. Bordeaux (RRI Frontiers of Life). L.A. and V.W. thank Dr. N. Martin and Dr. E. Ducrot for access to confocal microscopy, Dr. J.P Chapel for help with DLS measurements.

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How to model frictional contacts in sheared and active colloids?

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In colloidal systems, the role of frictional contacts has been largely ignored. However, recent evidence indicates that friction between colloids can significantly impact their behavior, particularly if the relative velocities between adjacent colloids is high, for example in the presence of shear forces or in the context of active matter systems. Typical models utilized to describe colloid friction have been adapted from those originally developed in the field of granular materials. These models have been combined with standard translational and rotational additive white noise terms, analogous to those used for particles without frictional contacts. While this approach may be sufficient for describing a multitude of phenomena, it is thermodynamically inconsistent from a fundamental perspective. Models that account for fluctuations as a counterpart of Stokes drag but not for the additional fluctuations that necessarily arise as a counterpart of frictional contacts may be in violation of Onsager relations and may not obey the fluctuation-dissipation theorem in the equilibrium limit.

In the present talk, we demonstrate how to develop a thermodynamically consistent model of colloidal matter with frictional contacts. We show that thermodynamic inconsistency due to the consideration of incomplete thermal fluctuations can (incorrectly) lead to the prediction of different equilibrium temperature values for the rotational and translational degrees of freedom, which are both different from the bath temperature. This leads to a new generalized class of dissipative particle dynamics (DPD) thermostats with rotational-translation coupling. Additionally, we present effects of frictional contacts using the example of Poiseuille flow and motility induced phase separation (MIPS) in active Langevin particles.

Defect formation in an expanding ensemble of spinners

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Ensembles of spinners are representative class of active systems. A particular case is that of magnetic droplets driven by a rotating field [1], where a polycrystal is formed with a row of disclinations decorating the grain boundary. Here we use a 2D model of repulsive spinners interacting by viscous vortical flows to study the dynamics of the ordering of the ensemble. Interestingly, the ordering of the ensemble takes place only if repulsion between the spinners is present. The ratio of the variance of the distance between nearest neighbors and its mean value (the Lindemann criterium) at the transition to the ordered state is close to the values found in systems with thermal noise.

The radial and azimuthal velocities which play an important role in the formation of the ordered structure and the dynamics of the defects are calculated. In the final state the numbers of positive N+ and negative N- disclinations satisfy the topological constraint N+-N-=6 (see Figure 1).

Keywords: spinners, disclination,Lindemann criterium

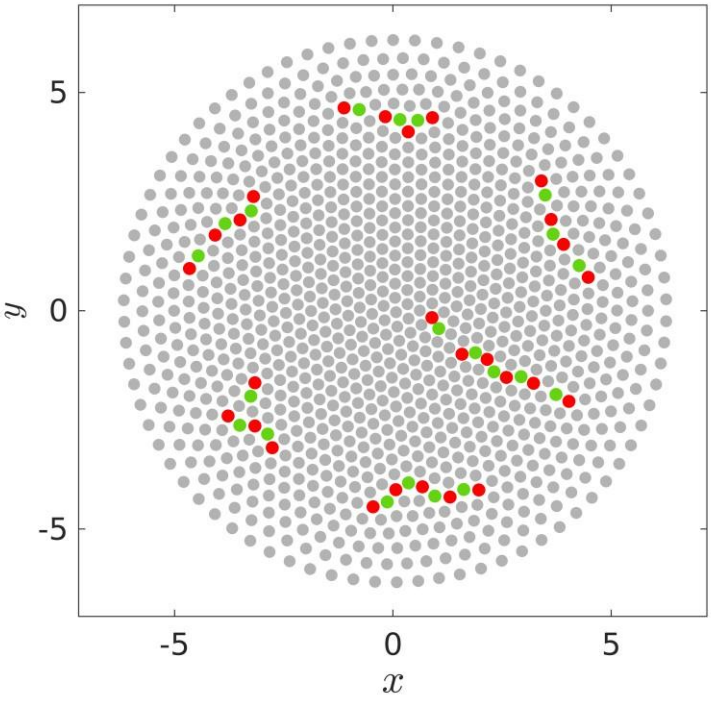

Figure 1. *Final stage of ensemble with hexagonal order. Red particle has 5 neighbors, green 7, gray 6.*

$\boldsymbol{N_+}$

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The effects of knot topology on the collapse of active polymers

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We use numerical simulations to study tangentially active flexible ring polymers with different knot topologies. Simple, unknotted active rings display a collapse transition upon increasing the degree of polymerization. We find that topology has a significant effect on the polymer size at which the collapse takes place, with twist knots collapsing earlier than torus knots. We rationalize this behavior as a consequence of the propensity for non-neighboring bonds of torus knots to be aligned with each other, thus avoiding collisions that would eventually lead to a MIPS-like collapse.

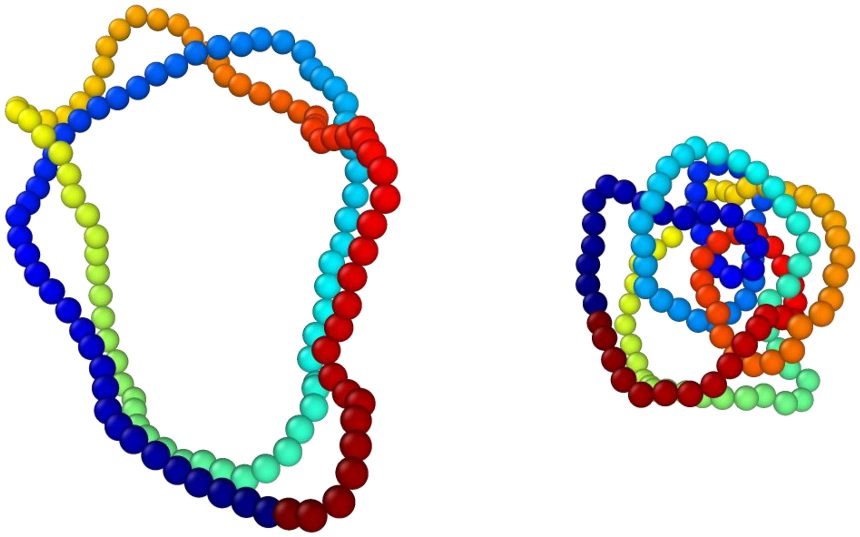

Figure 1. Torus knots (left: a trefoil) allow for longer active polymers to keep an open conformations while twist knots (right: a 4_1) collapse.

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 particles 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 result in the formation of 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.

Keywords: Active Brownian particle, chemotaxis, environmental memory, target search

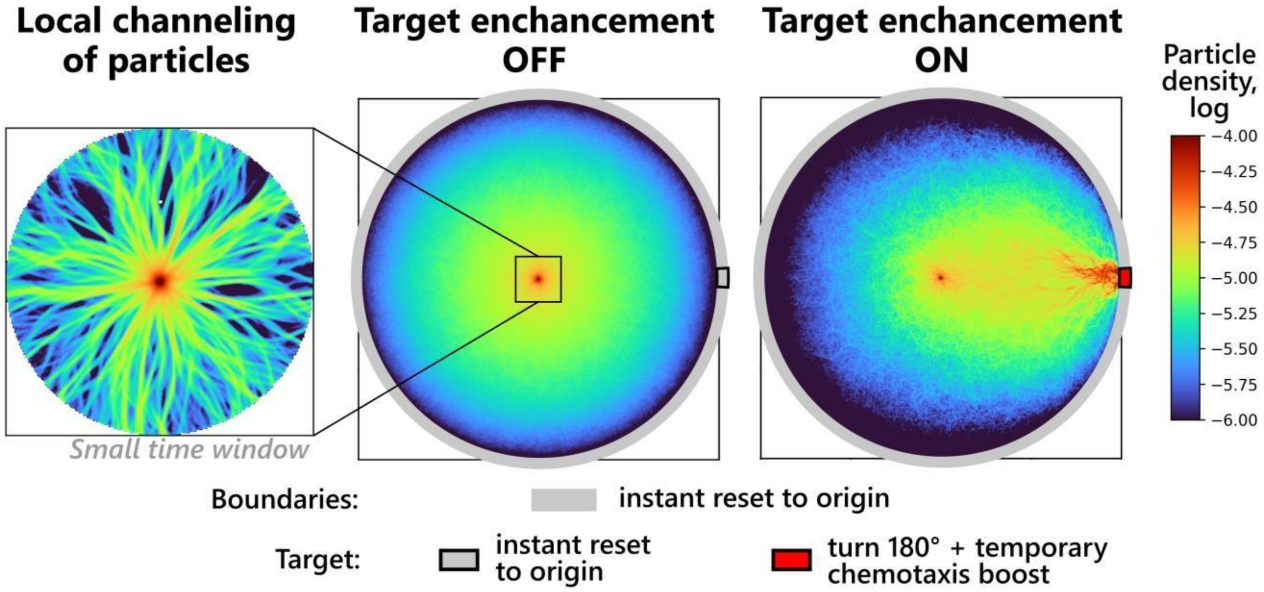

Figure 1. *Particle density distributions for a small arena (left), for large arena without specific target (center), and for reinforcement of a 5° target (right). Target reinforcement leads to symmetry breaking towards target and increases number of target hits by one order of magnitude.*

Generalized Fluctuation Dissipation Relations for Active Field Theories

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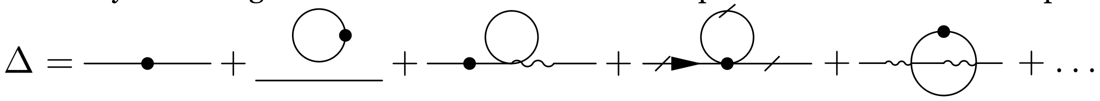
Breakdown of time-reversal symmetry is a defining property of non-equilibrium systems, such as active matter, which is composed of units that consume energy. We employ a formalism that allows us to derive a class of identities associated with the time-reversal transformation in non-equilibrium field theories, in the spirit of Ward-Takahashi identities. In [1], we present a generalization of the fluctuation-dissipation theorem valid for active systems as a particular realization of such an identity. Our approach relies on the response field (or MSR-DJ) formalism. It allows for calculating both the correlation function $C_{ab}(x,t)$ and linear response function $\chi_{ab}(x,t)$ of a physical field $\phi_a(x,t)$ using pathintegral methods by introducing an auxiliary variable, the "response-field" $\phi\tilde{}_a(x,t)$. We derive out-of-equiblibrium fluctuation dissipation relations, such as

$$\chi_{ab}(\boldsymbol{q},\omega) - \chi_{ab}(-\boldsymbol{q},-\omega) - i\omega\beta\, C_{ab}(\boldsymbol{q},\omega) = \Gamma \left\langle \varphi_a(-\boldsymbol{q},-\omega) i\tilde{\varphi}_b(\boldsymbol{q},\omega) \left(e^{-S[\varphi]} - 1\right) \right\rangle \equiv \Delta_{a\tilde{b}}.$$

We then apply these results to the Non-Reciprocal Cahn-Hilliard model for which we verify the identity via a graphical summation method. By treating the entropy S as an interaction term, we get a sum of Feynman diagrams for the deviation from the equilibrium fluctuation dissipation theorem:



The field theoretical toolbox developed here helps to quantify the degree of nonequilibrium activity of complex systems exhibiting collective behavior.

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Introduction of New Rotational Mini-Rheometer for Scarce Sample

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We introduce a miniaturized stress-controlled rheometer, aimed at enhancing rotational rheometry for analysis of scarce samples. This innovative device addresses the critical need for analyzing samples, such as biofilms, nascent drug formulations, and rare metal inks for microelectronics, which are typically limited in quantity due to their high production costs, challenging synthesis, or exclusive origins. Rheological measurements typically require at least 20 µl of sample material using commercial rotation rheometer, a requirement significantly reduced by our device, whereas the employed cone-plate geometry only requires 2 µl of sample material, representing a significant advancement in sample conservation. The mini-rheometer, approximately the size of a 50mm cube, utilizes an air bearing rotor made of quartz glass, manufactured via Selective Laser Etching (SLE). This subtractive 3D printing method for glass ensures the precision needed for an air bearing with µm-scale gaps. An outer magnetic field drives a centrally-placed magnet, while the angular displacement is accurately gauged by two Hall effect sensors, that detect the rotational movement of the inner magnet. The mini-rheometer´s efficiency and functionality were tested on calibration fluids, from water to viscous oils, as well as biological samples, such as percolating blood. This development extends the benefits of rotational rheometry – such as a wide range of strain rates and homogeneous strain profiles – to experiments where sample availability is limited. Due to the device´s miniaturized dimensions common, inverted microscopes can be used to study microstructural properties related to macroscopic flow behavior, which we used for the biological samples.

Keywords: mini-rheometer, scarce sample, Selective Laser Etching

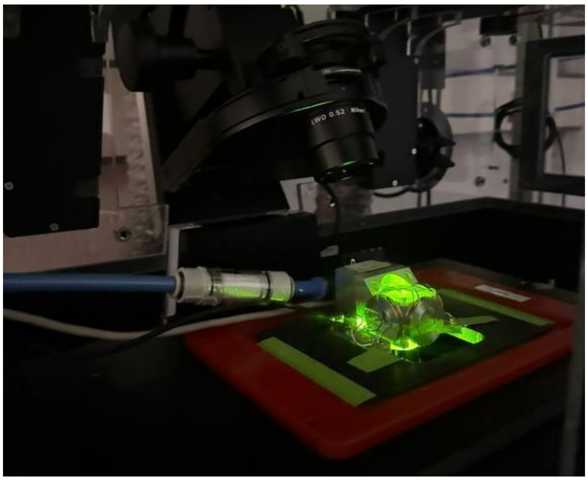

Figure 1. *Mini-rheometer on to of a fluorescence microscope.*

Advanced extensional rheometry on a rotational rheometer platform

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Performing extensional measurements with a rotational rheometer has proven successful for polymer melts with counter-rotating drums geometries. We describe new techniques to extend the limits of existing devices at low extensional stresses and large Hencky strains, and show the importance of simultaneous sample visualization to ensure truly uniform extensional deformation. The use of a second motor for measurements with dual counter-rotating drums can significantly improve the torque sensitivity and thus extends the measuring range to lower extensional rates, samples with lower viscosity and smaller sample sizes. By moving one of the drums in vertical direction during extensional deformation, the sample is tilted slightly, overlapping after one revolution is avoided and increased maximum deformations is achieved. Compared to standard operation, where the maximum Hencky strain is limited to 4, Hencky strains of over 8 were achieved. Additional optical access to the measurement setup throughout the experiment allows validation of the inclination angle.

Simultaneous visualization of the sample and image analyses reveal that overshoots in the extensional viscosity of the measured polymer melts are often attributable to necking.

By equipping the rheometer with a lower linear drive and combining the setup with a highspeed camera, capillary breakup experiments can be carried out on liquids with low viscosity. The rapid movement made possible by the linear drive and an optimized optical setup are required to perform these measurements at a level that previously required a separate device. In combination with the standard rotational drive of the rheometer, it is possible to shear the sample prior to stretching or to investigate torsional properties of viscoelastic liquid bridges.

The use of polarized imaging, which visualizes the stress distribution of the samples during elongation by measuring the local birefringence over the entire sample area, provides further insight into the various applications discussed.

Keywords: Extensional rheology, capillary breakup, polarized imaging

Physical mechanisms of MetaParticle-membrane interaction

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Nanoparticles (NPs) are promising drug carriers [1] across diverse biomedical applications, including targeted cancer therapies, diagnostic imaging and advanced vaccines. However, the clinical translation of nanocarriers remains limited due to complex biological barriers that reduce cellular uptake and therapeutic efficacy. The core composition and ligand conformations significantly influence their ability to overcome these barriers. Traditionally, coarse-grained models represent NPs as rigid beads, failing to incorporate the intrinsic plasticity that arises from corona formation and flexible cores. This leads to a limited understanding of the cellular uptake mechanism. Here, we introduce a coarse-grained NP model designed to capture the inherent flexibility of nanoparticles, termed "MetaParticles" (MPs) [2]. First, we investigate how MP size, topology and internal arrangements govern their mechanical properties. Next, we investigate the physical mechanisms of MP-membrane interactions by placing a MetaParticle in the proximity of a coarsegrained lipid membrane. We analyze the impact of nanocarrier flexibility on membrane binding, deformation, cellular uptake and potential translocation pathways.

Our results show that, in bulk, MP diffusivity correlates with size, while the mechanical properties are determined by topology and internal structure. In the proximity of a membrane, specific interactions induce distinct uptake mechanisms, including bending and fast endocytosis, suggesting distinct mechanisms for enhanced cellular entry specific for our MPs.

This framework represents a significant advance in developing adaptable, flexible nanocarriers and promises to inform the design of next-generation drug delivery systems and materials with broad applications in biomedical engineering and soft matter.

Keywords: Metaparticle, Membrane, Drug delivery, Soft matter, Modelling, Biophysics

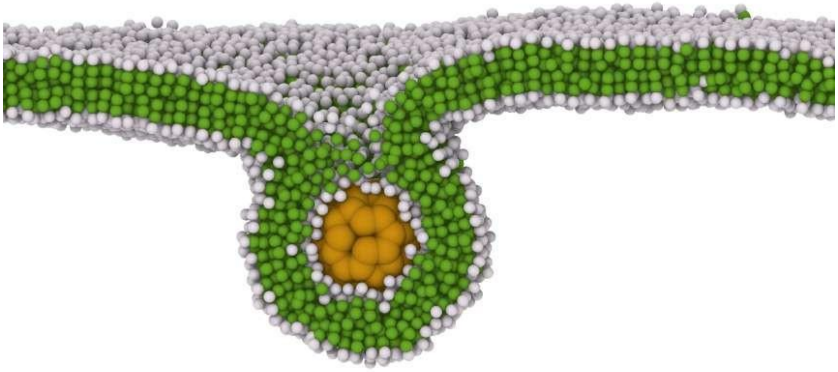

Figure 1. *MP60 encapsulation process, demonstrating passive diffusion in coarse-grained membrane.*

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Dynamics of Systems with Many Immiscible Fluids

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Interactions between multiple immiscible fluid components occur frequently in natural and industrial processes. For instance, the dynamics of injected CO2 with water and oil is critical for enhanced oil recovery [1], and the generation of emulsion droplets [2] consisting of oils and other fluids has applications in the medical, cosmetic and food industries. Additionally, lubricant coatings on surfaces, exploited by pitcher plants, can help to repel liquid droplets and exhibits self-healing properties [3]. Despite the prevalence of these multicomponent systems, models that can accurately capture the dynamics of an arbitrary number of immiscible fluids remain lacking. A critical bottleneck is the problem of reduction consistency [4], whereby a N component system must reproduce the N-1 component system when one fluid is absent.

In our work, we develop a fully reduction consistent numerical scheme capable of simulating dynamic fluid systems with no limitations on the number of components. Enabled by these new developments, we demonstrate how the classic four colour theorem can explain key physics in phase separation processes. Finally, we investigate applications including three component droplet emulsion generation and patterned lubricated surfaces.

Keywords: Fluid Dynamics, Droplets, Microfluidics, Phase Separation

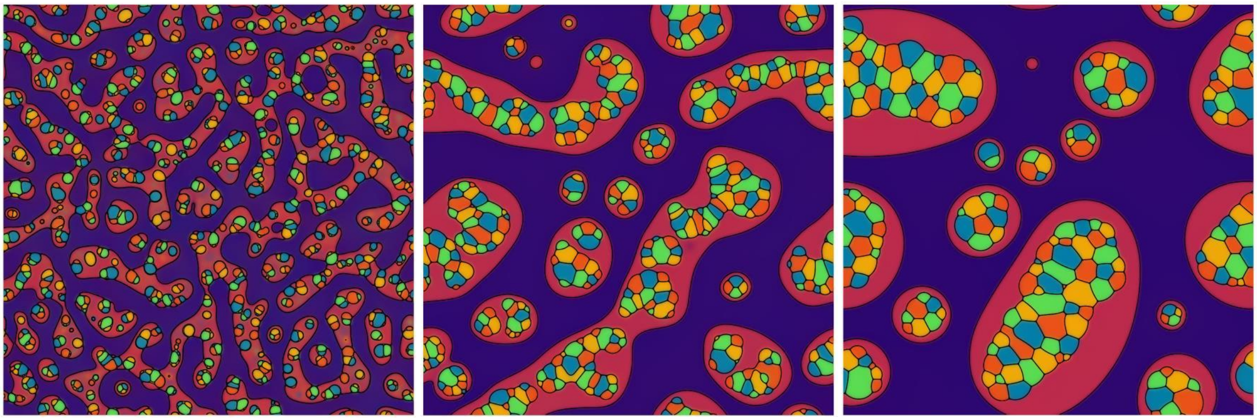

Figure 1. *Snapshots of phase separation process with six immiscible fluid components. Interfacial tensions have been selected such that the presence of the red component is energetically favorable at the interface of the purple component. We observe two distinct isolated coarsening regimes in the same system.*

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Machine Learning many-body potentials for charged colloidal Suspensions

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The Derjaguin-Landau-Verwey-Overbeek (DLVO) theory has been remarkably successful in describing the phase behavior of charge-stabilized colloids in solution. However, it fails to explain phenomena that suggest attractive interactions between like-charged colloids, particularly in low-salt solutions [1]. Simulations can give insight into these interactions. Unfortunately, simulations of charged colloidal suspensions with explicit ions, known as primitive model simulations, are computationally intensive. To overcome this challenge, we use machine learning (ML) techniques to develop an effective coarse-grained many-body potential for charged colloids, thereby eliminating the need to simulate explicitly the ions in solution, as illustrated in Fig. 1. We construct these effective many-body potentials by expressing them as a function of all colloid coordinates, using a set of two-body and three-body symmetry functions, and fitting them with a simple linear regression scheme.

Using these ML potentials significantly accelerates the simulations while providing new insights into the intriguing 'like-charge attractions' observed between colloids in solution. In this study, we present the framework for developing these effective potentials and compare them to other potentials used to describe suspensions of charged colloids.

Additionally, we investigate the gas-liquid and gas-solid coexistence behavior that can arise as a result of colloidal 'like-charge attractions', specifically in simulations employing ML potentials. Our simulations reveal that phase coexistences found in low-charge electrolytes cannot be directly extrapolated to high-charge electrolytes, a conclusion that contrasts with predictions based on Poisson-Boltzmann theories [2].

Keywords: Machine Learning, Charged Colloids

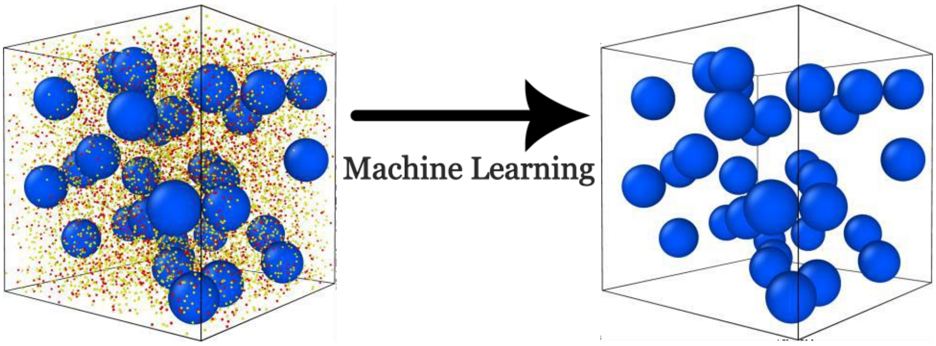

Figure 1. *Using a machine learning framework we generate a coarse-grained many-body potential, eliminating the need to explicitly consider ions in colloidal suspension when performing simulations.*

Acknowledgements: T.R.t.R. and M.D. acknowledge funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. ERC-2019-ADG 884902 SoftML).

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Bayesian Design of Hydrophobic Bio-Based Foams

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With the growing demand for sustainable materials, bio-based foams have emerged as a viable alternative to petroleum-derived counterparts. However, their sensitivity to moisture remains a significant limitation to broader practical application [1–2]. Developing hydrophobic bio-based foams without compromising mechanical integrity is a complex challenge, requiring a careful balance between material composition and performance. In this study, we employ Bayesian optimization to systematically enhance the hydrophobicity of methylcellulose-based foams while preserving structural integrity. By incorporating hydrophobic agents such as lignin, citric acid, precipitated calcium carbonate, and graphite, we tailor the foam properties through a data-driven, computationally guided approach [3]. The initial contact angle on the developed bio-foam samples has been improved from 110° to 160° through the addition of these agents.

A key challenge in this optimization lies in the high-dimensional nature of the formulation space. Multiple compositional variables influence both hydrophobicity and mechanical performance in a non-linear way. Traditional trial-and-error methods are impractical due to the complexity and cost of experimental synthesis. This makes an intelligent optimization strategy essential. By leveraging a Bayesian optimization framework, we efficiently explore this multidimensional and non-convex landscape, identifying an optimal multi-additive composition that maximizes hydrophobicity while maintaining strength. Unlike the initial experimental dataset—where each foam formulation contained only methylcellulose and a single additive—the optimized formulation strategically integrates multiple components, leveraging potential synergistic effects to enhance performance.

This approach not only improves predictive accuracy but also significantly reduces experimental workload by limiting the number of required formulations. Instead of testing all combinations, the model focuses experimental efforts on the most promising candidates. This accelerates material discovery and conserves resources. The study demonstrates the power of machine learning-assisted material design in sustainable engineering and provides an efficient pathway for developing water-resistant bio-based foams, building on our prior research optimizing similar systems [4].

Keywords: Bio-based foams, Bayesian Optimization, Hydrophobicity, Mechanical Properties, Material Design

Acknowledgements: This work was supported by the Finnish Ministry of Education and Culture's Pilot for Doctoral Programmes (Pilot project Mathematics of Sensing, Imaging and Modelling).

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Friday 3rd October 2025

C. Colloidal matter

(Room 1)

Evolution of depletion forces during thermodynamic quenching and heating processes

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Depletion forces have gained significant scientific and technological interest due to their essential role in the determination of the phase behavior and self-assembly in colloidal and biological systems. While extensive studies have calculated these forces under equilibrium conditions using various theoretical, computational, and experimental methods, the understanding of the depletion forces under non-equilibrium thermodynamic conditions has been more limited and often relies on specific models and approximations. In this contribution, we report results on the evolution towards equilibrium of the depletion forces during quenching and heating processes. By applying a recent theoretical approach, based on the contraction of the bare forces, we account for the temporal evolution of the effective potentials for a bidisperse colloidal system made up of soft spheres subjected to a temperature protocol, revealing long-range interactions that arise from the evolution through non-equilibrium states.

Keywords: depletion potential, entropic forces, colloidal binary mixtures, thermal evolution

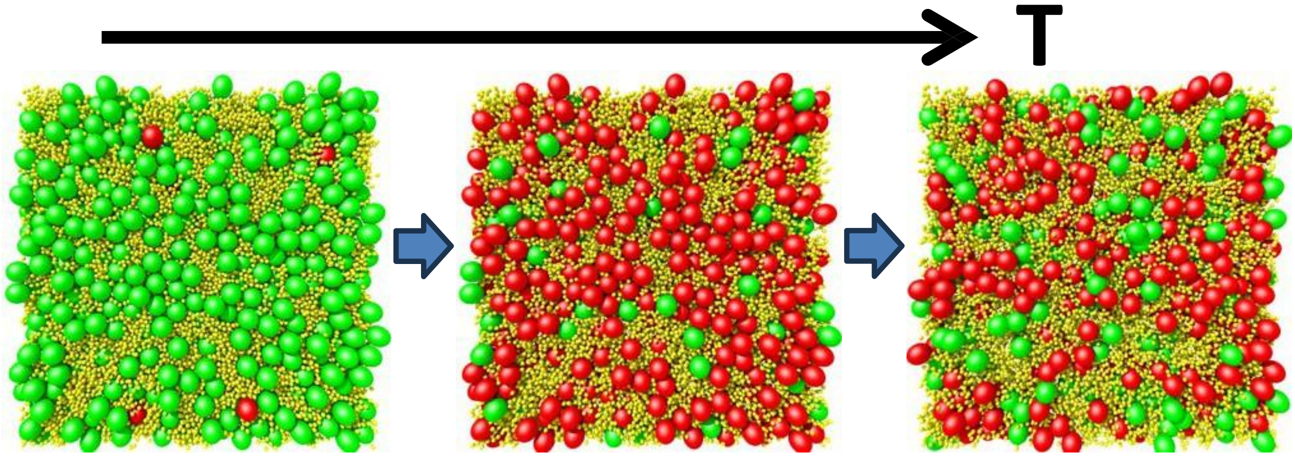

Figure 1. *Evolution of the colloidal binary mixture by increasing the temperature, as indicated by the arrow.*

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Surface Charged Polymeric Micelles - A model system to switch between steric and electrostatic interactions

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We investigate surface charged micelles in aqueous solution formed by carboxy terminated n-octacosyl-poly(ethylene oxide) block copolymers, C-PEO5-COOH with 5 the PEO molar mass in kg/mol, by small angle neutron scattering (SANS), zeta-potential measurements, DLS and rheology. The -COOH end group was introduced by selective oxidation of the CH_3OH end group of a C-PEO5-OH precursor using Bobbitt's salt. Micellar solutions of different concentrations in the dilute and semidilute range were investigated at pH 2, 6 and 12 to vary ionic strength and the number of effective surface charges Z. Using in addition mixtures of C-PEO5-COOH and C-PEO5-OH, in total Z was tunable between $0<Z<145$ by pH and mixing ratios.

SANS measurements reveal that the intramicellar form factor is identical at the different pH-values which implies that the individual micellar structure is unaffected by the number of surface charges. On the contrary, the intermicellar structure factor and the phase behavior show a strong dependence on Z. In particular, we observe a distinct shift of the liquid - fcc crystal phase boundary. A quantitative analysis in terms of a screened Hard Sphere Yukawa potential reveals a very good agreement between experiment and theory without adjustable parameters.

Because of this consistency and of the tunability of the n-alkyl-PEO starlike micelles, we consider this system to be an excellent model for further studies on the interplay between steric and electrostatic interactions in soft colloids.

Keywords: Charged Colloids, SANS, Rheology

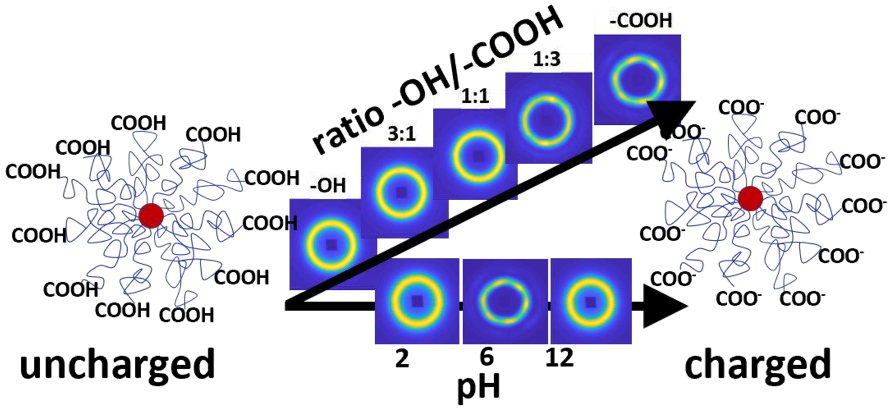

Figure 1. *The number of surface charges can be adjusted by pH and mixing ratio.*

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Probing cage dynamics in concentrated hard sphere suspensions and glasses with high frequency rheometry

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We probe the evolution of cage formation and shear elasticity with increasing volume fraction in hard sphere suspensions, with emphasis on the short-time dynamics. We utilize linear viscoelastic (LVE) measurements, by means of conventional rotational rheometers and a home-made HF piezo-rheometer, to probe the dynamic response over a broad range of volume fractions up to the very dense glassy regime in proximity to random close packing. We focus on the LVE spectra and times shorter than those corresponding to the dynamic shear modulus G_0 plateau, where the system approaches transient localization and cage confinement. At these short times (higher frequencies), a dynamic cage has not yet fully developed and particles are not (strictly) transiently localized. This corresponds to an effective solid-to-liquid transition in the LVE spectrum (dynamic moduli) marked by a high frequency (HF) crossover. On the other hand, as the volume fraction increases caging becomes tighter, particles become more localized, and the onset of the localization time scale becomes shorter. This onset of transient localization to shorter times shifts the HF crossover to higher values. Therefore, the study of the dependence of the HF crossover properties (frequency and moduli) on volume fractions provides direct insights concerning the onset of particle in-cage motion and allows direct comparison with current theoretical models. We compare the experimental data with predictions of a microscopic statistical mechanical theory where qualitative and quantitative agreements are found. Findings include the discovery of microscopic mechanisms for the crossover between the two exponential dependences of the onset of the localization time scale and the elastic shear modulus at high volume fractions as a consequence of emergent many body structural correlations and their consequences on dynamic constraints. Moreover, an analytic derivation of the relationship between the high frequency localized short- time scale and the elastic shear modulus is provided which offers new physical insights and explains why these two variables are experimentally observed to exhibit nearly-identical behaviors.

Keywords: cage dynamics, high frequency rheology, microscopic theory

Acknowledgements: support from the Twinning project FORGREENSOFT (Number: 101078989 under HORIZON WIDERA-2021-ACCESS-03) and US Army Research Office via a MURI grant with Contract No. W911NF-21-0146.

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Examining the micromechanics of rough colloidal gels

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Colloidal gels are viscoelastic materials that are used in applications from food to soft robotics. At small strains, these gels can be characterized by elastic system spanning networks. The system fluidifies with increasing applied stress. Previous work showed that by modifying the microscale structure of the gels through the utilization of "rough" particles, one could create gels with enhanced toughness, and thus a delayed transition from elastic to plastic behavior [1,2]. In this work we investigate the microstructural network interactions in thermo-reversible rough particle gels that delay the onset of plasticity. Using a high speed "rheo-confocal" microscope we capture changes in the systems bulk properties and microstructure simultaneously.

Keywords: Networks, Colloidel Gels, Plasticity

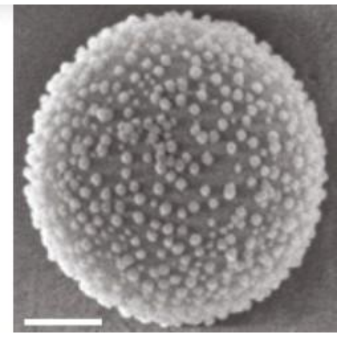

Figure 1. *Scanning electron microscope image of a rough colloidal particle. Rough particles are synthesized by modifying the surface topology of a silica core with the addition of small asperity particles. The scale bar represents 200 nm. This figure is modified from Fig.2 of Reference 2.*

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Molecular Simulation of Dielectric and Assembly Properties in Grafted Nanoparticle–Polymer Nanocomposites

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Dielectric materials are integral to communication devices such as smartphones and personal computers. Previous research has shown that the dielectric performance of materials can be enhanced by adding nanoparticles to polymer melts (1). Recently, polymer-grafted nanoparticles have attracted much attention due to their unique optical and electronic properties. In this simulation study, we aim to improve and understand the dielectric performance of nanocomposite materials by modelling a variety of polymer-grafted nanoparticles.

We used a particle-based model for the polymer grafted nanoparticles, using polyimide as the reference polymer to determine the degree of coarseness and system size. Figure 1 shows the variation of the dielectric tangent with frequency for the GNP model and the number of grafted polymers in this study. In the high-frequency band (100 MHz) of Figure 1, a difference in the dielectric loss tangent due to the number of polymers was observed. This is thought to be due to the dispersion of GNPs as the number of grafted polymers increases. In this study, we discuss the aggregation behavior of GNPs and the change in the dielectric loss tangent when the nanocomposites are subjected to an electric field.

Keywords: Molecular simulation, graft polymers, polyme r nanocomposites, dielectric materials

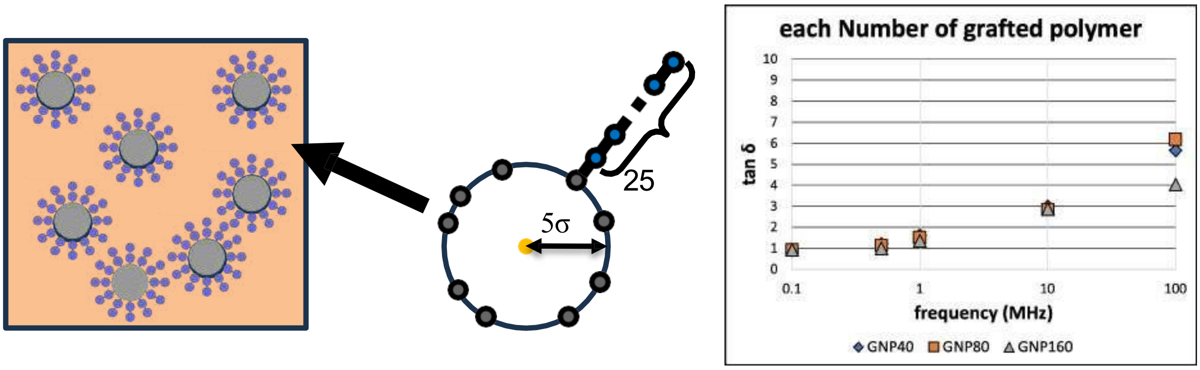

Figure 1. *Simulation model of nanocomposite system Dielectoric loss (tan δ) of each number of grafted polymer NPs.*

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Friday 3rd October 2025

I. Interfaces, surfaces, membranes, emulsions

(Room 2)

Unveiling the Role of Wall Transparency in Wetting and Capillary Phenomena

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Atomically thin walls are becoming increasingly prevalent in modern technologies, offering unique properties which set them apart from conventional materials. One of their most intriguing characteristics is the transparency to interparticle interactions, a phenomenon that has been demonstrated to impact processes as diverse as wetting [1], capacitive energy storage [2], electron transfer [3], and fluid flows [4,5]. However, the influence of wall transparency on wetting and capillary phenomena remains poorly understood. In this contribution, we explore how van der Waals interactions across thin solid walls affect capillarity and substrate wetting [6]. We find that a fluid-filled, sidewise-open channel beneath a thin wall can drastically enhance the apparent hydrophobicity of the wall, effectively converting hydrophilic materials into hydrophobic ones. In addition, a fluid covering a thin wall can either suppress or promote capillary condensation, depending on whether it is in the vapor or liquid state, leading to the emergence of unusual capillary phases within the channel. These findings demonstrate the transformative potential of wall transparency in designing and manipulating interfacial phenomena.

Keywords: Interfacial phenomena; wetting; capillary condensation superhydrophobicity; graphene; wall transparency; atomically thin walls

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Hollow polymeric particles as opacifying agents for TiO_2 replacement in coatings

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Metal oxides, particularly titanium dioxide (TiO_2), are widely used as pigments and opacifying agents in various industries, among them paints, food, and cosmetics. Global demand for TiO_2 is projected to reach approximately 8 million tonnes this year, with paints and coatings accounting for the largest share (~55%). However, TiO_2 production imposes a significant environmental burden due to its high CO_2 emissions and large carbon footprint. This has driven the search for alternative materials with lower environmental impact, though full replacement of TiO_2 remains challenging.

In this study, we explore the potential of hollow 3-(trimethoxysilyl)propyl methacrylate (TPM) particles as a substitute for TiO_2 in coatings. We employ hollow particles (HP) with different size and core-to-shell ratio, incorporating them into coating formulations alongside film-forming polymer particles. By adjusting interparticle electrostatic interactions and drying conditions, we can tune the final distribution of hollow particles within the film, and therefore the optical properties of the coating. Our results demonstrate that HP-containing coatings exhibit excellent light reflectance, outperforming TiO_2-containing reference coatings (Figure 1).

Keywords: Coatings, Opacifiers, Hollow particles, Reflectance

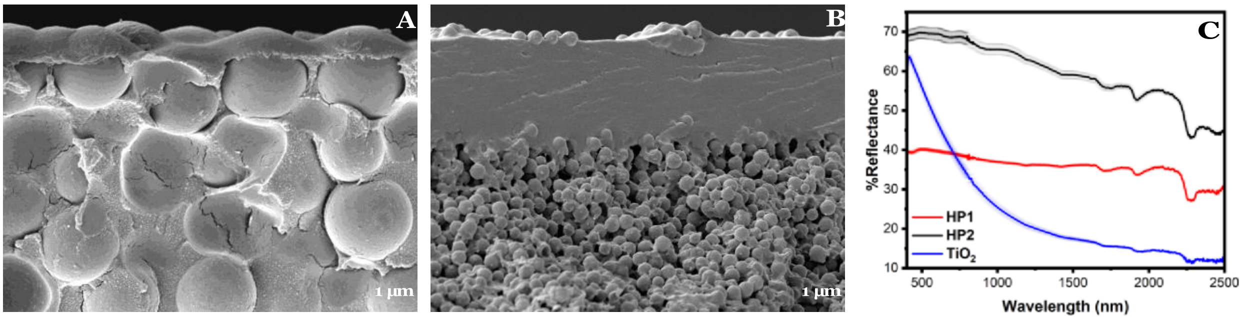

Figure 1. *Cross-sectional SEM micrographs of coatings dried at 25 °C and 50% relative humidity. The coatings contain negatively charged latex and (A) HP1 or (B) HP2 with 5 µm diameter and 0.3 µm shell thickness, or 1 µm diameter and 0.25 µm shell thickness respectively. (C) presents the % light reflectance of the coatings versus a TiO_2 reference coating.*

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Swelling-induced patterning in soft microchannels

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We study the effect of inflation on the swelling-induced wrinkling of thin elastic membranes in a set-up that is commonly used to create microchannels in lab-on-chip applications. Using a combination of experiments and associated numerical simulations, we demonstrate that the outofplane deformation of the inflated membrane and the resulting anisotropic stress lead to two distinct instabilities as the swelling progresses. The membrane first develops small-amplitude wrinkles that retain the cross-channel symmetry. Their wavelength depends on the pressure and is set in a process similar to the axisymmetric buckling of pressurised, uni-axially compressed cylindrical shells [1]. As swelling increases, the membrane undergoes a secondary instability during which the wrinkles coarsen into large-amplitude folds whose morphology can be controlled by the degree of preinflation. We elucidate the fundamental mechanisms responsible for this behaviour and explain how inflation can be used as a control mechanism in the manufacture of layer-stack microchannels [2], which are capable of conveying fluids at large pressures, and are therefore useful in mixing, flow focusing and particle sorting applications. Earlier works have already demonstrated benefits of using swelling for designing and manufacturing of patterned microchannels over more traditional methods in which the channel shape is 'frozen' early in the production [3]. Our study suggests new opportunities for robustly producing corrugated microchannels by providing a pathway to a range of patterns that are otherwise inaccessible.

Keywords: swelling-induced wrinkling; patterned microchannel; lab-on-chip application

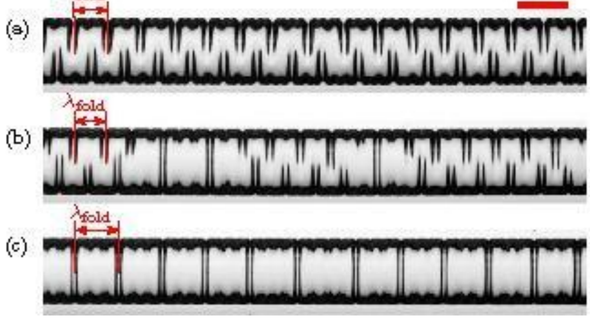

Figure 1. *Representative wrinkling patterns observed in experiments with soft microchannels, where a thin membrane serves as the top wall. The membrane was inflated under constant pressures of (a) 493 Pa, (b) 1020 Pa, and (c) 1259 Pa, followed by swelling.*

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Droplet Impact and Spreading on Superhydrophobic/Superamphiphobic Surfaces with Re-entrant Structures

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Re-entrant pillars have a strong capability to repel droplets of liquids in comparison with regular pillars. Nevertheless, there has been little insight into how the key structural parameters of reentrant pillars influence the dynamics of impacting droplets. In this work, we have carried out numerical simulations and experimental studies to portray the fundamental physical phenomena that can explain the alteration of the surface wettability from adjusting the design parameters of the doubly re-entrant pillars (Figure 1), for example. We demonstrate that the behaviours of droplets can be manipulated by altering the dimension and pitch of the re-entrant pillars. Further, hydrophobizing the pillars allows the droplet to bounce off the surface at a faster rate. Nonetheless, once the impacting pressure exceeds the breakthrough pressure, the droplet will penetrate the interstices of the doubly re-entrant pillars regardless of being hydrophobized. This requires further understanding of how the design parameters can be optimised to facilitate sustainable droplet bouncing.

Keywords: Wetting, Droplet Impact, Re-entrant Pillars

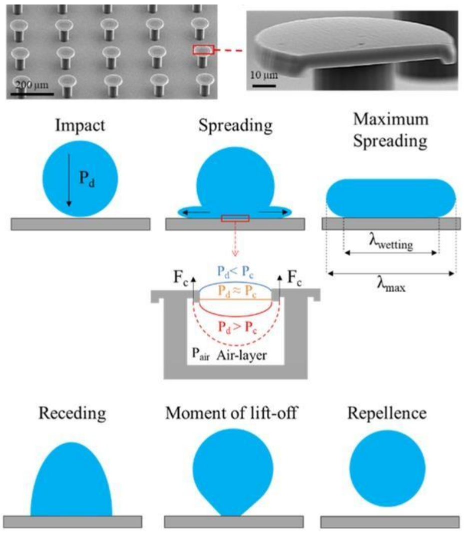

Figure 1. *Doubly re-entrant pillars with a cross-sectional view and the relevant droplet impact process.*

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Shear-Rate Dependence of the Surface Tension of Glass-Forming Fluids

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By using Molecular Dynamics simulations, we study the surface properties of glassforming fluids showing non-Newtonian rheology. While the viscosity of these fluids typically depends strongly on temperature and density, the surface tension is often assumed to be simply a constant.
Nevertheless some recent experiments have shown that the measurement of the surface tension of viscoelastic fluids is far from trivial, showing pronounced hysteresis effects.
By applying shear flow in the interface, we detect that the surface tension depends on the shear rate. We connect this to the regime of shear-thinning and nonNewtonian rheology of the bulk fluid. Importantly, the standard way of determining surface tension from the pressure drop across the interface gives rise to an effective surface tension in the non-Newtonian fluid that mixes bulk and interface properties. We show how the pressure anisotropy can be used to clearly define the bulk and interface regions and extract a genuine shear-rate dependent surface tension. The talk will be concluded by an investigation of the relaxation time of the surface tension, when shear is applied.

Keywords: Surface Tension, Molecular-Dynamics simulations, Interfaces

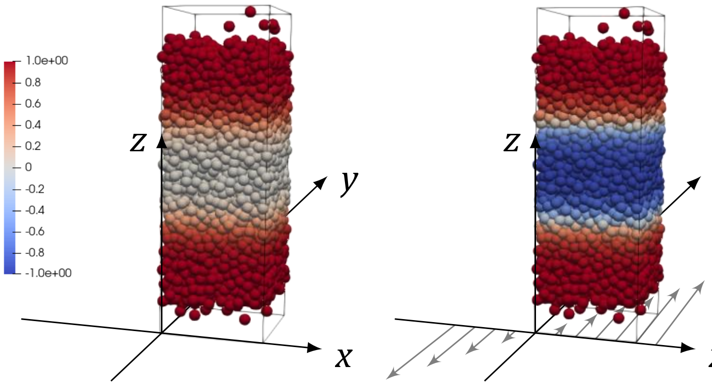

Figure 1. *Snapshots of the simulation setup without (left) and with (right) imposed shear.*

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Friday 3rd October 2025

BF. Biomedical & Food applications

(Room 3)

3D Printable Aqueous Two-Phase Systems for Tissue Engineering

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The restricted porosity of most hydrogels established for in vitro three-dimensional (3D) tissue engineering applications limits embedded cells with regard to their physiological spreading, proliferation, and migration behavior. To overcome these confines, porous hydrogels derived from aqueous two-phase systems (ATPS) are an interesting alternative. However, while developing hydrogels with trapped pores is widespread, the design of bicontinuous hydrogels is still challenging.

We discuss an ATPS consisting of photocrosslinkable gelatin methacryloyl (GelMA) and dextran. The phase behavior, monophasic or biphasic, is tuned via the pH and dextran concentration. This allows the formation of hydrogels with a bicontinuous structure with interconnected-pores. The pore size can be tuned from ca. 4 to 100 µm.
Cytocompatibility of the hydrogels is confirmed by testing the viability of stromal and tumor cells. Their distribution and growth pattern are cell-type specific but are also strongly defined by the microstructure of the hydrogel.

Furthermore, we demonstrate that the bicontinuous porous structure is sustained when processing the system in 3D printing. Improving the performance of the aqueous two-phase system during the printing process can be achieved via an in-situ acidification reaction combined with an in-line optical detection of the phase separation as well as by controlling rheological properties via the addition of a 3rd polymer component.

Keywords: Aqueous Two-Phase Systems, Tissue engineering, hydrogel, 3D printing

Assessment of lipid nanoparticles as carriers for magnetic resonance imaging contrast agents

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Due to the reduced number of available positive (T_1) contrast agents (CAs) for magnetic resonance imaging (MRI) and possible health risks of some Gd-chelates, alternative CAs are being searched and developed. The promising approach is the use of nanoparticulated systems in different ways eg: (1) formation of inorganic NPs with paramagnetic ion incorporated into a nanostructured framework; (2) formation of hybrid constructs consisting of inorganic and organic components, with paramagnetic functionality either in inorganic or organic part; (3) formation of "nano-co-assemblies" of organic components with paramagnetic functionality at least in one. Nanoparticle-based CAs have gained significant attention over the past few decades [1]. Among these, more and more attention is paid to lipid-based ones serving as carriers for the contrast-providing entity. These lipid-based carriers enhance physicochemical stability, biocompatibility, and intracellular uptake of formed CAs and can potentially improve relaxivity (r_1) [2].

The paper will present the potential of glyceryl monooleate-based lipid nanoparticles, focusing on the formation of hybrid constructs of lipid liquid crystalline nanoparticles with common paramagnetic oxides that possess both hydrophilic and hydrophobic characteristics (LLCNPs@Gd_2O_3 and MnO). It will also discuss the formation of nanoassemblies using Gd-chelating lipids (LLCNPs@Gd-DTPA-BSA). This assessment will show the physicochemical and biological properties of prepared constructs, highlighting the relation between the type of developed lipid nanoparticles and the high relaxation rates they achieve. A certain focus will be given to studies on paramagnetic ion loading efficiency, including calculations per nanoparticle, paramagnetic ion release in different conditions, and, finally, cell uptake from prepared lipid-based nanoparticles as MRI CAs, which are critical characteristics regarding the development of CAs for MRI. The conclusion of the presented research is that these lipid-based systems are considered innovative and biologically safe MRI T_1-enhancing contrast agents for future *in vivo* imaging.

Keywords: glyceryl monooleate, Gd-chelating lipid, nanoassemblies, hybrid nanoparticles, gadolinium oxide, manganese oxide

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Tuning Cellulose Microfibrill Containing Plant-Protein Gels by Shear

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Cellulose microfibrils (CMFs), derived from plants waste material offer a unique fibrillar structure [1] and serve as sustainable, natural and functional ingredients for dietary-rich, clean-label food products contributing to the texture and stability of these products. [2,3] However, the dispersion of CMFs is challenging due to their tendency to aggregate via OH-driven hydrogen bonding and van der Waals interactions. [4] While previous studies demonstrate that high-energy treatments of CMF dispersions in the presence of biopolymers improves homogeneity and reduces aggregation, the role of processing conditions in controlling these interactions and the resulting microstructural changes remains underexplored. [1,4] Understanding the influence of shear induced microstructural changes in these composite systems is crucial to tailor the texture of plant-based food products.

This study investigates the impact of processing conditions on the rheological and structural properties of composite CMF plant-protein systems. Model systems were prepared by dispersing CMF in presence of plant-proteins, followed by controlled shear treatments using a Microfluidizer varying the applied energy density. The findings demonstrate that alternating the processing conditions significantly influence the structural and rheological properties of CMF – plant-protein systems. These results provide a foundation for tailoring the continuous phase in plant-based food systems, optimizing texture and mouthfeel.

Keywords: Cellulose, Plant-protein, Shear-tuning, High-pressure homogenization

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Tuning β-lactoglobulin/lactoferrin complex coacervate properties via solvent quality modification

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Heteroprotein complex coacervation (HPCC) refers to associative liquid-liquid phase separation occurring between two or more proteins. HPCC is primarily driven by electrostatic interaction (enthalpic contribution) and counterions release (entropic contribution). Its physicochemical properties, largely influenced by electrostatic interaction strength, can be modulated via pH and ionic strength. A promising yet underexplored approach to tuning coacervation is altering solvent quality, specifically the dielectric constant (ε) of the medium [1]. Electrostatic interactions between a single cation and anion is described by the Coulomb energy ($E = -e^2/4\ \pi\varepsilon_0\varepsilon\ \sigma$) where e is the elementary charge of the ions, σ is the separation distance between the ions, and ε_0 is the dielectric permittivity of a vacuum.

β-lactoglobulin (βLG) and lactoferrin (LF) are known to form complex coacervates [2]. Here, we investigated HPCC between these two globular whey proteins in water/glycerol mixtures. The linear viscoelasticity of βLG/LF coacervates, prepared at pH 5.6, was examined as a function of temperature (T = 5–40°C) and glycerol content (0-40%). The thermal behavior was investigated using differential scanning calorimetry (DSC).

Results showed a significant increase in the storage (G′) and loss (G′′) moduli with increasing glycerol content. The time-temperature superposition (TTS) principle applied to all βLG/LF coacervate systems, and TTS data were fitted to the Fractional Maxwell model. Activation energies (E_a), calculated using the Arrhenius equation, increased with glycerol content, indicating strengthening of the electrostatic interactions since E_a represents the activation barrier that needs to be overcome to dissociate an ionic pair within βLG/LF coacervates. DSC further revealed a freezing point shift to negative temperatures as a function of glycerol content.

This study demonstrates that solvent quality can effectively tune the rheological and thermal properties of HPCC, offering potential for diverse applications.

Keywords: Heteroprotein complex coacervation, Linear viscoelasticity, Time temperature superposition, Electrostatic interactions.

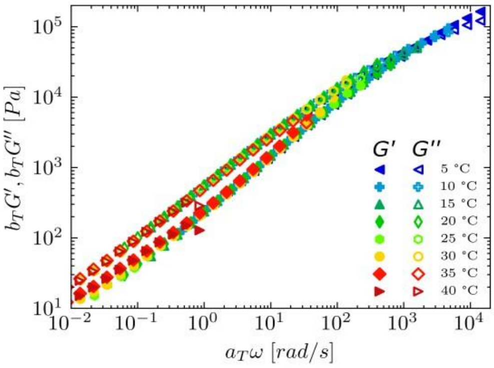

Figure 1. *Time Temperature Superposition principle applied to βLG/LF coacervates prepared in 30% glycerol.*

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Structuring the meat-like structures in plant-based meat analogues: A comprehensive multiscale study by small angle scattering

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Driven by growing concerns over health, sustainability, and ethical practices, the transition to a plant-based diet makes plant-based meat analogues (PBMAs) more mainstream [1]. For the production of anisotropic fibrous meat-like structures, high moisture extrusion cooking (HMEC) is used extensively in industry. The mechanism of the structural anisotropy formation is however unknown due to the 'black-box' characteristics of the extrusion process, and the complexity of the multi-component system. To address this, an in situ small-angle neutron scattering (SANS) measurement during HMEC was executed with a customized cooling die. The results propose the chain-like arrangement of protein nano-aggregates, fractures of the viscoelastic mass, and sharp temperature-dependent solidification as new theories [2]. Building upon this, we investigated the role of dietary fibers (DFs) in enhancing structural anisotropy by combining SANS with scanning small-angle X-ray scattering based imaging (sSAXS), which can access a wide length scale covering from nanometer to millimeter, and large sample area. The added DFs were found to form celluloserich regions, which created many protein-cellulose interfaces, ultimately provoking crack initiation and thus more fibrous structures [3]. Our study provides valuable insights into PBMA structuring by integrating advanced neutron and X-ray scattering techniques, bridging soft matter physics with food science. This work introduces a novel experimental setup and techniques for investigating hierarchical bio-based materials, with potential applications in functional biomaterials and sustainable food design.

Keywords: plant-based meat analogues, fibrous structure, high-moisture extrusion cooking, mall angle scattering

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Breaking the Law (of Darcy): Espresso Flow at High Pressure

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Brewing espresso offers a rich physical system for studying fluid flow through porous media under pressure. In this process, hot water is forced through a compacted bed of ground coffee, often modelled using Darcy's law, which predicts a linear relationship between pressure and flow rate. However, coffee is a complex porous medium which reacts to flow both mechanically and chemically, swelling, dissolving and reconfiguring during brewing. In addition, real-world brewing conditions typically involve high pressures (6–11 bar), raising questions about the validity of simple Darcy models under these conditions.

We present new experimental measurements, as well as a theoretical model describing the pressure–flow relationship in espresso extraction. We observed that at low pressures (2–6 bar), the flow rate increases linearly with pressure, consistent with Darcy-like behaviour. At higher pressures (>6 bar), however, the flow rate saturates and even slightly decreases, indicating a deviation from Darcy's law. We argue that this nonlinearity may arise from microstructural changes in the coffee bed under mechanical stress, such as pore collapse or compaction[1-2].

Our findings suggest that standard models of porous media might be insufficient to describe flow at high brewing pressures. The results motivate the development of new constitutive models tailored to espresso extraction and deepen our understanding of pressure-driven transport in deformable and reactive granular media.

Keywords: porous media, nonlinear pressure–flow relationship, espresso extraction, Darcy's law, reactive flows

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Friday 3rd October 2025

F. Fluid Dynamics and Rheology

(Room 4)

How do glasses yield?

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One way to tell fluids from glasses is through the deformation behavior: Glasses yield under application of a large enough external force, the static yield stress. Conversely, glasses that flow do so only at the expense of a minimum stress, limited by below through the dynamic yield stress. Since stress is a tensorial concept, a full description of yielding involves a discussion of the influence of different deformation modes. The yielding point thus becomes an entire yield surface in the space of principal stresses. However, so far not many theory or simulation studies of glass-forming fluids consider flow geometries beyond simple shear. We argue that investigation of different yielding geometries will reveal further insight into the microscopic mechanisms behind glassy dynamics.

We present simulation results for glass-forming Lennard-Jones mixtures under continuous deformation in different geometries, from tension to shear to compression [1]. From the stressstrainrate relations (the flow curves), we extract the dynamical yield stresses around the modecoupling theory transition temperature. The resulting yield surface challenges the theoretical understanding of the glass transition through common theoretical models: We show how this can be boiled down to the question of whether glasses are stronger in tension or in compression. The question is related to details of the interactions that might become relevant when contrasting simple glass-forming models with more realistic interaction potentials derived using machine learning [2].

Keywords: glass transition, rheology, yield stress, computer simulation

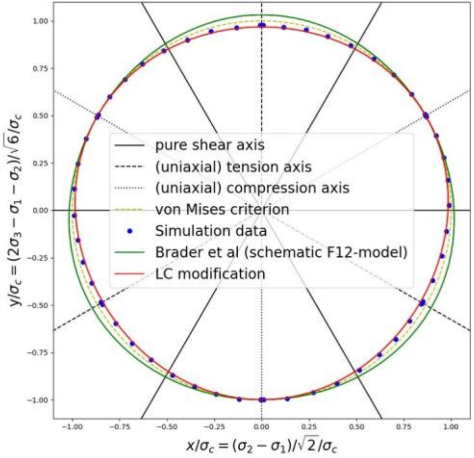

Figure 1. *Yield surface of a glass-forming Lennard-Jones mixture. Simulation data (symbols) are compared to a standard prediction of mode-coupling theory (green line) and deviate qualitatively. A modified MCT model captures the simulation data well. [1]*

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Nanorheology of Magnetic Nanogels

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In the past decade, nano- and microgels have garnered significant attention due to their unique physical properties and promising medical and technological applications. Recent research has focused on incorporating magnetic nanoparticles (MNPs) into nanogels for targeted drug delivery, enhanced uptake by tumor cells, and advancements in medical imaging and therapy. The potential for remote control of the rheology and internal structure of these soft colloids with external stimuli, particularly magnetic fields, makes magnetic nanogels (MNGs) highly attractive for bio-compatible regulation. However, to fully unlock MNG-based applications, a deep understanding of magnetodynamics and rheology is vital.

We model MNG suspensions in a nanochannel using hybrid Molecular Dynamics—LatticeBoltzmann methods to solve coupled Langevin and Navier-Stokes equations [1]. The system features a laterally periodic slit geometry with shear flow via a moving top wall (see Fig. 1). External uniform magnetic fields, either constant ($H\vec{H}$) or rotating ($H\vec{H}_{rrrrrr}$), were applied.

First, we develop a viscosity measurement protocol similar to [2] and validate it against Einstein's viscosity equation. Second, we quantify MNG suspension viscosity under $H\vec{H}$ by varying concentrations, $H\vec{H}$ strength, and magnetic dipolar coupling of MNPs, revealing shear-thinning inherent to viscoelastic suspensions. We demonstrate that magnetic forces suppress shear-driven rotation in MNGs, increasing viscosity. Thirdly, halting the wall and applying $H\vec{H}_{rrrrrr}$ generates pure magnetically induced shear flow, producing zero net flow versus directed wall-driven shear, with distinct MNG deformation modes. This $H\vec{H}_{rrrrrr}$-induced shearing aligns with the negative viscosity concept proposed by Schliomis in 1994 for ferrofluids under AC magnetic fields [3].

Keywords: magnetic nanogels, viscoelasticity, negative viscosity, nanorheology

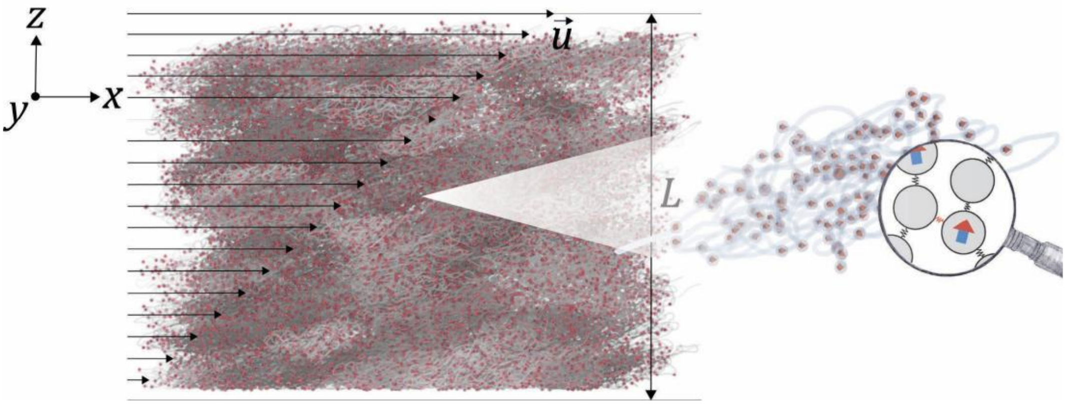

Figure 1. *Nanochannel containing sheared MNG suspension. (Inset) A single MNG, with polymer chains depicted as semi-transparent threads and embedded MNPs implicitly visualized.*

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Rolling, sliding and trapping of driven particles in square obstacle lattices

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Transport in complex and dynamic microscopic environments is fundamentally shaped by hydrodynamic interactions [1]. Specifically, microparticle transport is governed by a delicate interplay between shear forces arising from particle-substrate lubrication interactions, and pressure forces resulting from flow-field symmetry breaking. Here, we investigate the motion of externally driven, rotating particles near a substrate patterned with a square lattice of cylindrical obstacles, which serves as a model complex environment. Remarkably, we observe a reversal in the direction of particle motion as obstacle spacing decreases, revealing a sensitive competition between shear-induced forward rolling and pressure-driven backward sliding, as shown in Fig. 1. Furthermore, the direction of motion can be controlled by tuning the rotational frequency, as the pressure forces also have a vertical component that modifies the particle's height above the surface, thereby altering the shear force [2]. Finally, we find that a rotating particle rolling toward the lattice from outside can either penetrate the lattice or get scattered by it, depending on the rotational frequency, enabling activity-based particle sorting. Our results demonstrate how structured environments shape microscale transport and offer new strategies for microfluidic design, targeted cargo delivery, and tunable active materials.

Keywords: Microrollers, Particle sorting, Steerable particles.

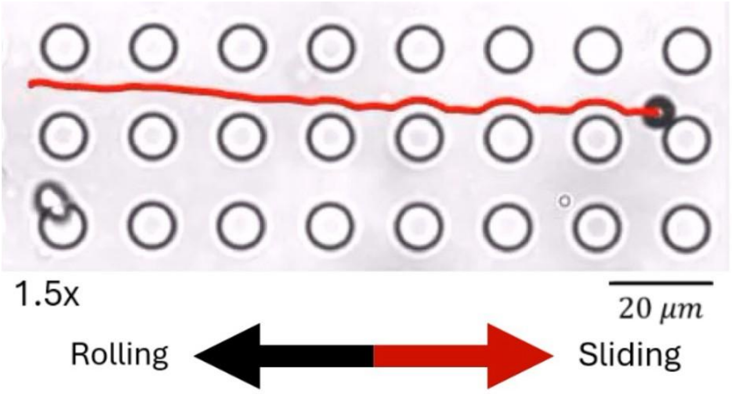

Figure 1. *A rotating particle within an obstacle lattice, sliding in the direction opposite to the rolling motion.*

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Boost, Contraction and Bands of Emulsion Flow

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The yielding transition underpins processes and technologies such as additive manufacturing, injection molding, food rheology, and oil transport [1]. It has been shown that this transition can be triggered by microroughness patterns on the walls of microfluidic channels [2]. These patterns induce local plastic rearrangements, reducing the material's viscosity and facilitating flow. In this study, we explore two asymmetrical geometries: herringbone-riblet and wedge-like grooves [3,4]. These textures introduce a topological asymmetry along the flow direction, influencing the fluidization process.

By increasing the pressure load, we provide insights into how wall boundary conditions affect the transition from solid-like to fluid-like behavior in yield-stress emulsions. Our findings demonstrate that these geometries activate selective fluidization, resulting in a measurable flow gain with respect to opposite directions along the channel axis. The herringbone pattern generates a layered flow banding across the channel cross-section, while the wedge-shaped grooves induce a uniform flow gain throughout the channel cross-section.

To complement the experimental results, we employ Lattice Boltzmann numerical simulations based on a two-dimensional model of directional roughness [5]. We provide a protocol to measure the stress profile within channels featuring asymmetric boundary conditions and provide evidence of a double rheological response. This integrated approach highlights the interplay between pressure, geometry, and flow behavior, offering valuable insights into yield-stress fluid manipulation.

Keywords: directional roughness; fluidization; microfluidic channel; emulsion; yield-stress-fluids

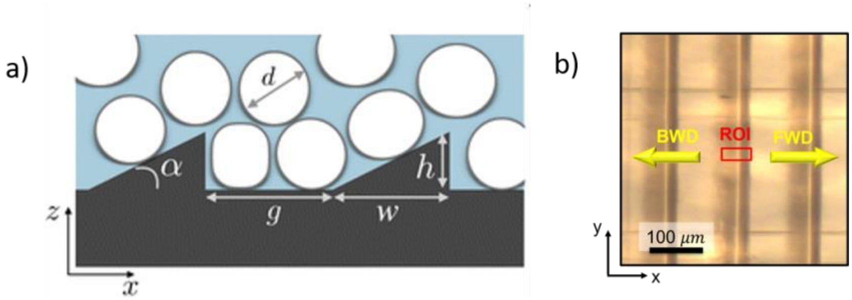

Figure 1. *(a) Side view sketch of the directional roughness consisting of wedge-shaped posts.*

(b) Top view of the wedged grooves realized by maskless photolithography.

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Elucidating the Physical Mechanisms of Foam Cleaning Efficiency

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The physical properties of liquid interfaces, drops, bubbles and foams have been shown to lead to efficient cleaning of solid surfaces [1]. Recent observations suggest that unstable liquid foams are particularly efficient in removing different kinds of surface contaminations [1,2], yet the underlying mechanisms remain to be elucidated. One hypothesis is that the continuous rearrangement of bubbles induces significant shear forces at the liquid-solid interface, capable to detach the contaminations, which are then removed by the absorption capacity of the foam. However, other effects, such as the direct action of the gas/liquid/solid triple line may also contribute.

To identify and quantify the dominant physical mechanisms responsible for the observed phenomena, we combine complementary experimental approaches for the removal of different kinds of model contaminations. These include fluorescently labelled lipid layers of controlled numbers of layers, human sebum or highly viscous materials. We exploit purpose-designed millifluidic chips to analyse the response of these surfaces to the flow of two-dimensional foams with well controlled properties (as shown in Figure 1), providing insight into the effect of macroscopic shear stresses exerted by the collective effect of bubbles. These foam scale experiments are combined with investigations of single-interface interactions with the model surfaces, allowing us to put in evidence the strong impact of direct triple line interactions. For this purpose, the millifluidic experiments are combined with dynamic contact angle measurements to quantify the mechanical stresses exerted by the liquid interface on the solid surface.

Our findings offer new perspectives on the complex interplay between macroscopic foam dynamics and localized gas/liquid/solid interactions, paving the way for optimizing foam-based cleaning processes.

Keywords: Cleaning foams, Multiphase interactions, phospholipids, contact line dynamics.

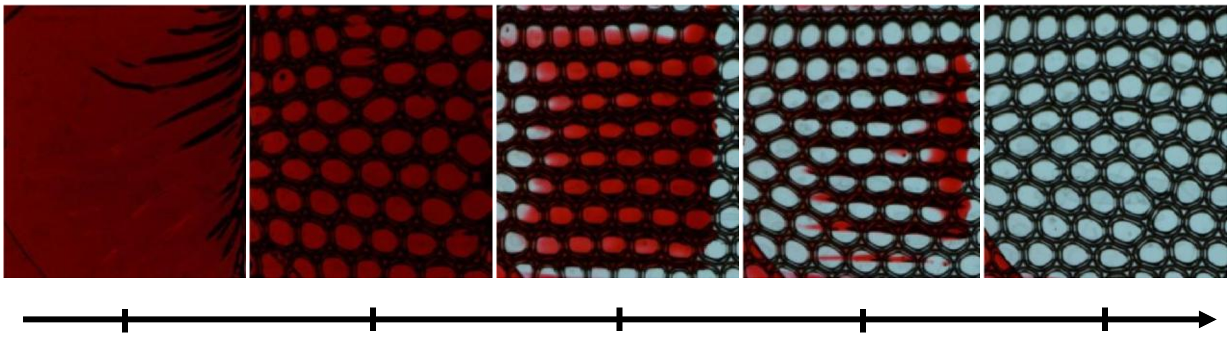

Figure 1. *2D foam flow applied on a viscous macroscopic contamination (red), showing its progressive removal.*

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Linear Viscoelasticity of Dilute Solutions of Semiflexible Polymers

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The linear viscoelastic response of dilute solutions of semiflexible polymers is studied using Brownian dynamics simulations of coarse-grained bead-spring chains. The springs obey the FENE Fraenkel force law, a bending potential is used to capture chain stiffness and hydrodynamic interactions are included through the Rotne-Prager-Yamakawa tensor. By calculating the relaxation modulus following a step strain, we demonstrate that the bead-spring chain behaves like an inextensible semiflexible rod over a wide time window with an appropriate choice of spring stiffness and chain extensibility. In the absence of hydrodynamic interactions, our results agree with the existing theoretical predictions for the linear viscoelastic response of free-draining, inextensible, semiflexible rods in dilute solutions. It is shown that at intermediate times, the stress relaxation modulus exhibits power law behaviour, with the exponent ranging from $-(1/2)$ for flexible chains to $-(5/4)$ for highly rigid chains. At long times, rigid chains undergo orientational relaxation, while flexible chains exhibit Rouse relaxation. Hydrodynamic interactions are found to effect the behaviour at intermediate and long times, with the difference from free-draining behaviour increasing with increasing chain flexibility. Computations of the frequency dependence of loss and storage moduli are found to be in good agreement with experimental data for a wide variety of systems involving semiflexible polymers of varying stiffness across a broad frequency range.

Keywords: Dilute Polymer Solutions, Semiflexible Polymers, Linear Viscoelasticity, Brownian Dynamics