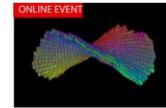


# Advanced School in Soft Condensed Matter Solutions in the Summer 2021

5 - 9 July 2021

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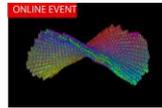


## Poster Programme

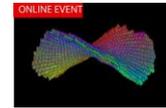
**Day 1 – Tuesday 6 July 2021**

**Virtual Poster Session 1: 16:25–17:55pm**

- P1.1 **Advection-induced pumping and mixing in active microchannels**  
Gonçalo Antunes, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Germany
- P1.2 **The role of the solvent and nonionic surfactant in the self-assembly of cellulose nanocrystals**  
David Attia, Ben-Gurion University of the Negev, Israel
- P1.3 **A new approach to the electrical conductivity theory for suspensions**  
Svitlana Balika, Odesa I. I. Mechnikov National University, Ukraine
- P1.4 **Command of active droplets by patterned topological defects and laser tweezers**  
Hend Baza, Kent State University, USA
- P1.5 **Imaging of biologically relevant lyotropic mesophases**  
Dominika Benkowska-Biernacka, Wrocław University of Science and Technology, Poland
- P1.6 **Boundary-interior principle for microbial navigation in complex geometries**  
Jan Cammann, Loughborough University, UK
- P1.7 **Phase transitions in a system with cluster-crystal formation**  
Rômulo Cenci, Universidade Federal de Santa Catarina (UFSC), Brazil
- P1.8 **Colloidal Particle Focusing and Sorting in Microchannels via Solute Concentration Gradients**  
Adnan Chakra, Loughborough University, UK
- P1.9 **Self-Propulsion in rigid and deformable biological objects through diffusiophoresis phenomena**  
Prabha Chuphal, Skolkovo Institute of Science and Technology (Skoltech), Russia
- P1.10 **Inverse design in trajectory space for nonequilibrium colloidal self-assembly**  
Avishek Das, University of California Berkeley, USA
- P1.11 **Dynamics of trapped artificial microswimmers in a shear flow**  
Tanwi Debnath, University of Calcutta, India
- P1.12 **Monomer aggregation and pretransitional ordering in DNA liquid crystals**  
Simone Di Leo, Università degli Studi di Milano, Italy
- P1.13 **Self assembled colloids and their aggregation in an anisotropic solvent**  
Devika Gireesan Sudha, University of California Merced, USA



- P1.14 The anomalous transport of tracers in an active bath**  
Omer Granek, Technion, Israel
- P1.15 Underscreening in concentrated electrolytes**  
Hannah Hayler, University of Oxford, UK
- P1.16 Effects of hybrid lipids on the structure of a model cellular membrane of mixed lipids**  
Prashant Hitaishi, Shiv Nadar University, India
- P1.17 Active Surfaces and Defect-Mediated Morphogenesis**  
Ludwig A Hoffmann, Leiden University, Netherlands
- P1.18 Defect Loops in Three-Dimensional Active Nematics as Active Multipoles**  
Alexander Houston, University of Warwick, UK
- P1.19 Cells moving against obstacles: the response of a drop of active matter to external forces**  
Aondoyima Ioratim-Uba, University of Bristol, UK



### P1.1 Advection-induced pumping and mixing in active microchannels

Gonçalo Antunes, Paolo Magaretti, Jens Harting and Siegfried Dietrich

Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Germany

Much attention is currently being given to the problem of manipulating fluids at the microscale. The resulting field of microfluidics has been applied successfully to fields such as 3D fabrication and biomedical research. In all these situations, fluid must be pumped in a controlled fashion, making micropumps a fundamental component of many microfluidic systems.

Moreover, controlling chemical reactions requires stirring solutions by means of micromixers. An intriguing technique to manipulate fluid flows in a channel is phoresis. In such a set up fluid flow is obtained upon imposing an inhomogeneous concentration of some solute, which generates flow in a boundary layer around the channel walls.

We perform simulations of active channels via a Lattice Boltzmann method coupled to a solver for an advection-diffusion equation for the solute concentration. In contrast with common methods for phoresis, our method does not assume a slip velocity at the walls, instead fully solving the dynamics of the boundary layer. We show that a chemically patterned active channel can act as a micropump even when it is fore-aft symmetric.

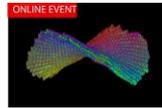
Analytical calculations further confirm the existence of pumping steady states. This is possible due to a spontaneous symmetry breaking occurring when advection rather than diffusion is the dominant method of solute transport. We further show how both geometrical and chemical inhomogeneities are required for pumping and how one may tune the flow rate. We go beyond the steady Stokes flow limit and obtain both steady flow and sustained oscillations with a frequency that can be tuned. Finally, we find that axisymmetry can also be broken, mixing the fluid even at steady state.

### P1.2 The role of the solvent and nonionic surfactant in the self-assembly of cellulose nanocrystals

David Attia and Rachel Yerushalmi-Rozen

Ben-Gurion University of the Negev, Israel

The self-assembly and phase behavior of cellulose nanocrystals (CNCs) in binary liquid mixtures of Ethylene-Glycol (EG): Water was investigated. CNCs are charged rigid-rod nanoparticles that exhibit first-order phase transition from isotropic suspension to chiral nematic ( $N^*$ ) liquid crystal (LC) phase above a critical volume fraction in aqueous suspensions. Our findings indicate that a small fraction of water delays the onset of colloidal jammed states previously reported in water-free organic solvents. Here the full phase diagram of CNCs evolves, including the  $N^*$  phase, characterized by long-range orientational order and non-isotropic macroscopic properties. Furthermore, the effect of the solvent-mixture composition on the properties of the CNCs mesophases is found to be scale-dependent: The micron-size pitch of the  $N^*$  phase *decreases* as the dielectric constant ( $\epsilon_r$ ) of the solvent mixture is *reduced* (higher EG content). Yet the nanometric inter-particle spacing of the CNCs rods (measured using SAXS and cryo-TEM) is almost independent of the EG content. These observations may be rationalized by hypothesizing that vicinal water, adsorbed at the CNCs surface, prevent kinetic arrest, dictate the local  $\epsilon_r$  and thus the effective diameter of the rods (via the Debye length), while  $\epsilon_r$  of the liquid-mixture dominate the pitch length (micron scale) and the optical



properties. The findings indicate that the water content of EG: Water mixtures may be used for engineering colloidal inks where delayed kinetic arrest and jamming of the CNCs enable printing and casting of tunable, optically active thin films and coatings.

Following these findings, the study was extended to the investigation mixtures of nonionic surfactant, single-walled carbon nanotubes (SWNTs) and CNCs. The observations indicate that the 4-component system (SWNTs-CNCs-surfactant-water) organizes by forming a network of surfactant-dispersed SWNTs that co-exists with the CNCs mesophases, where the surfactant molecules mediate the interactions and lead to the formation of a hybrid.

### **P1.3 A new approach to the electrical conductivity theory for suspensions**

Svitlana Balika

Odesa I. I. Mechnikov National University, Ukraine

The electrical conductivity  $\sigma$  of suspensions exhibits [1,2] different types of behaviour, depending on the surface potential, structure of the electrical double layer (EDL), ion mobilities and concentrations, and other factors. The existing (classical Maxwell-Garnett, cell, or electrokinetic) models for  $\sigma$  are often unsatisfactory, for they involve a number of unjustified assumptions about the microstructure of the system and ignore strong electromagnetic interaction between its constituents. In this work, we present, based on recent results [3,4], a new approach to the problem which suggests that the electrical conductivity of a real suspension can be expressed in terms of the parameters of a model dispersion obtained by embedding hard-core-penetrable-shell spheres into a uniform medium. The shells are assumed to be electrically inhomogeneous, characterized by a radial conductivity profile, and obey the rule of dominance for overlapping regions that the local conductivity is determined by the distance to the nearest particle. Such an approach enables us to investigate how the electric and geometric parameters of different parts of the EDLs contribute to the formation of the conductivity  $\sigma$  and predict different types of the functional dependence of  $\sigma$  upon the concentration of the particles. Testing the theory by contrasting its results with experimental data for concentrated suspensions of transparent particles (ghosts) [1] and latex particles [2] gives good results.

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### **P1.4 Command of active droplets by patterned topological defects and laser tweezers**

Hend Baza, Yuhan Wang, Hao Wang and Oleg Lavrentovich

Kent State University, USA

Nematic liquid crystal environment enables directional propulsion of spherical droplets representing aqueous dispersion of bacterial microswimmers<sup>1</sup>. Here we explore how the dynamics of active droplets can be controlled by patterning the nematic environment with nonsingular director field. We use the plasmonic metamasks technique to pattern the director in the form of non-singular disclinations. We demonstrate that interactions of the active droplet with the director gradients of the environment can be used to control the propagation direction, speed, and locations of traps



that stop propulsion. However, the manipulation of colloids in liquid crystals by laser tweezers is known for decades, the inclusion of living organisms provides limitations on the laser wavelength and power. Here, we use an azobenzene dye that has a trans-to-cis photoisomerization in the visible range that causes melting of the nematic phase with a low-power laser at room temperature and enables us to move the droplets and reorient their motility. Using 2D patterned nematic LCs and laser tweezers, one can guide the active droplets along complex routes with predefined points of residence.

The work is supported by NSF grant number DMR-1905053 and the Office of Sciences, Department of Energy, grant number DE-SC0019105.

- [1] Rajabi, M., Baza, H., Turiv, T. & Lavrentovich, O. D. Directional self-locomotion of active droplets enabled by nematic environment. *Nature Physics* 17, 260–266, doi:10.1038/s41567-020-01055-5 (2021).

### **P1.5 Imaging of biologically relevant lyotropic mesophases**

Dominika Benkowska-Biernacka and Katarzyna Matczyszyn Wrocław University of Science and Technology, Poland

There has been a growing interest in research on lyotropic liquid crystals (LLCs) of biological importance. Rod-like molecules, such as lipids, DNA or collagen, tend to self-organize into mesophases at a certain concentration and temperature. Furthermore, the examples of LLCs can be found in many complex biological structures, for instance, in cell membrane and myelin sheath [1-3].

In this study, we present formation and analysis of artificial myelin figures (MFs) consisted of a single type of zwitterionic phospholipids with luminescent dopants. Using the polarized light microscope equipped with a retardation plate allow us to detect the existence of liquid crystalline phases and to obtain information about the orientational order of lipids within multilamellar structures. Additionally, we demonstrate a detailed investigation of MFs performed by confocal fluorescence microscopy and two-photon fluorescence microscopy.

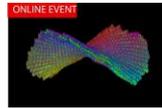
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[3] M. Mitov, *Cholesteric liquid crystals in living matter, Soft Matter*, 13, 4176-4209, 2017

### **P1.6 Boundary-interior principle for microbial navigation in complex geometries**

Jan Cammann, Fabian Jan Schwarzendahl, Tanya Ostapenko, Danylo Lavrentovich, Oliver Bäumchen and Marco G. Mazza

Loughborough University, UK

In recent years, biological microswimmers have attracted considerable interest due to the biological and ecological implications of understanding the mechanisms governing their dynamics. The possibility to harness their motion to power microdevices is a topic of exceptional importance for



modern microtechnology. When the motion of a motile cell is observed closely, it appears erratic, and yet the combination of nonequilibrium forces and surfaces can produce striking examples of organization in microbial systems. Most of our current understanding is based on bulk systems or idealized geometries, it remains elusive how and at which length scale self-organization emerges in complex geometries. We use experiments, analytical and numerical calculations to study the motion of motile cells under controlled microfluidic conditions, and demonstrate that probability flux loops organize active motion even at the level of a single cell exploring an isolated compartment of nontrivial geometry. By accounting for the interplay of activity and interfacial forces, we find that the boundary's curvature determines the nonequilibrium probability fluxes of the motion. We theoretically predict a universal relation between fluxes and global geometric properties that is directly confirmed by experiments. Our results represent a general description of the structure of nonequilibrium fluxes down at the single cell level opening the possibility to decipher the most probable trajectories of motile cells and may enable the design of geometries guiding the time averaged motion of microswimmers.

### **P1.7 Phase transitions in a system with cluster-crystal formation**

Rômulo Cenci

Universidade Federal de Santa Catarina (UFSC), Brazil

We studied the phase transitions that occur in crystals of agglomerates in two-dimensional systems. Simulating Brownian particles interacting through a repulsive soft-core potential, called Generalized Exponential Model ( $GEM\alpha$ ), and given by  $\exp(-\alpha r)$ , we find different types of phase transitions and characterize their nature as the density varies, for one choice of the parameter  $\alpha$ . A very interesting feature of this model is that, although it has an exclusively repulsive interaction at any distance, for low temperatures the model can form spatial patterns allowed by the soft-core nature of the potential, forming the so-called cluster-crystals. We simulate the thermodynamic equilibrium of the system using Langevin dynamics and parallel tempering techniques. To analyze the system, we also need use cluster analysis techniques such as Agglomerative Hierarchical Clustering. In order to explore the phase transitions that occur in the system, we measure thermodynamic properties such as the caloric curve, specific heat capacity and also the positional and orientational order parameters, as well as their corresponding correlation functions. Exploring the nature of each phase, either crystalline, hexatic or liquid, we find evidence of two of the main melting scenarios proposed in the literature, which are: the two-step melting scenario described by the KTHNY theory in the single particle regime; and a single step scenario with a first order phase transition between the cluster-crystal and the fluid, without the presence of an intermediate hexatic phase between the solid and liquid phases. In addition, we also explore isostructural transitions between the different crystalline phases of the system.



## P1.8 Colloidal Particle Focusing and Sorting in Microchannels via Solute Concentration Gradients Anjan Chakra, Guido Bolognesi, Naval Singh and Goran Vladislavjevic

Loughborough University, UK

An increasing interest in harnessing chemical energy in the form of solute concentration gradients has led to the exploration of colloidal particle manipulation by diffusiophoresis (DP) and diffusioosmosis (DO) in microfluidic devices (MFDs) [1]. In this study, we report a novel phenomenon that enables the pre-concentration and sorting of colloidal particles dispersed in a continuous flow within a straight microchannel (Figure 1). A bespoke  $\Psi$ -junction MFD is used to generate a steady-state salt concentration gradient perpendicular to the flow (Figure 1a). As a result, charged colloidal particles dispersed in the inner solution accumulate into two symmetric regions of the channel by forming two distinct focusing peaks at the junction. Downstream the channel, these peaks converge towards the centre while their intensity increases in which a particle focusing of ca. 60% is achieved (Figure 1b). This particle manipulation strategy can be easily controlled by adjusting the salinity level of the outer solution and can be exploited to sort particles based on their charge. Despite a similar colloid behaviour being reported in previous studies with a similar flow configuration [2], our experiments show that the observed particle dynamics is driven by a novel unreported physical mechanism, that combines DO, DP and hydrodynamic effects. The proposed method offers great potential for microfluidic bio-analytical testing and filtration applications.

Keywords: Electrokinetic Flows, Diffusiophoresis, Colloids, Microfluidics

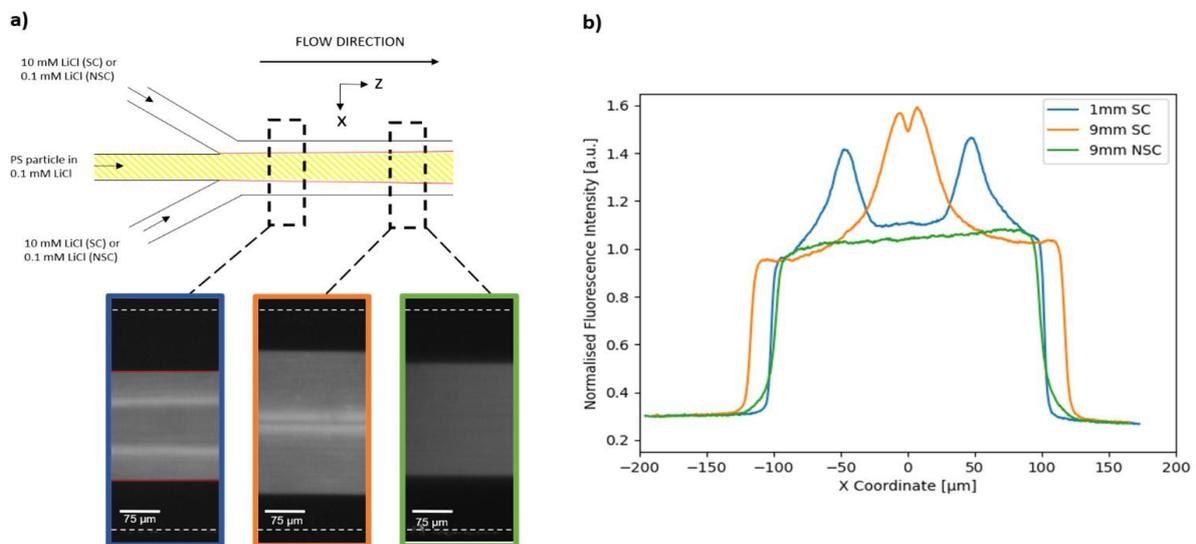
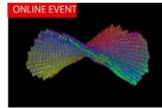


Figure 1: a) Schematic of the MFD with focused images obtained at 1 mm (blue) and 9 mm (orange & green) away from the junction, b) Normalised Intensity profile of colloids at distances specified in a). 'SC' and 'NSC' denote salt contrast and no salt contrast, respectively.

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## **P1.9 Self-Propulsion in rigid and deformable biological objects through diffusiophoresis Phenomena**

Prabha Chuphal and Snigdha Thakur

Skolkovo Institute of Science and Technology (Skoltech), Russia

Active matter systems stay far from equilibrium and traditionally studied in the context of biology and defined as being composed of active units or agents that continually convert ambient, stored, biological, or chemical energy locally into motion. Examples of active matter systems in Nature are schools of fish, flocks of birds, bacteria, self-organizing bio-polymers such as microtubules and actin etc., which ranges from macroscopic to microscopic length scale. Self-propelling systems are examples of active matter systems where self-propulsion associated with any biological species is essential for their functions such as transportation of materials, targeted drug delivery, growth of bacterial colonies, etc. These examples motivate us to study the active self-propelling systems. In our work, we focus on the modeling of synthetic objects that achieve self-motility under symmetry breaking. With the help of computational tools and statistical methods, we try to understand the self-propulsion of a deformable vesicle and colloidal particles using a coarse-grained simulation technique.

The work I will present is divided into two parts. Studies of the first part are motivated by cell motility. A simpler model for a membranous vesicle, that is chemically powered deformable active vesicle is studied with the help of a diffusiophoresis mechanism. The motion of an active vesicle in bulk system as well as in the presence of external flow exhibits different modes of propulsion and shape transformations depending on various physical parameters and environmental conditions. The dynamics of this deformable entity has been shown to change remarkably. The second part accommodates the chemotactic response of inert colloidal particles in the presence of chemically active colloid. This includes the diffusiophoretic capture of an inert colloid to the surface of a fixed/moving active colloid and the formation of moving clusters starting from Brownian particles. The local symmetry breaking is exploited to understand the self-propulsion.

## **P1.10 Inverse design in trajectory space for nonequilibrium colloidal self-assembly**

Avishek Das and David T Limmer

University of California Berkeley, USA

Predictively directing colloidal self-assembly has seen enormous experimental and theoretical interest due to the independent tunability of size, shape and interactions in colloids and nanoparticles. Design principles thus found are mostly applicable to systems in thermal equilibrium or relaxing to one. This is because equilibrium probability measures are of a Boltzmann form and hence can be modulated by changing the energetic stability of target structures. These approaches cannot predict the transient dynamics of self-assembly and also fail to apply to systems driven by external dissipative forces to a nonequilibrium steady-state. However, far-from-equilibrium assembly environments are the norm in biological systems and also exploited ubiquitously in manufacturing protocols for soft materials. A general framework for predicting design principles in nonequilibrium steady-states is currently lacking.



We demonstrate that nonequilibrium molecular dynamics trajectories conditioned on assembling into a target structure encode a set of optimal interactions and driving forces resulting from a variational principle in the driven trajectory ensemble. We have developed an optimization algorithm to solve this variational problem with explicitly evaluated stochastic gradients in design-space. We have used this algorithm to find general rules for the self-assembly of DNA-labeled colloids in a shear flow, for various target structures and dynamical phases [1]. We discover optimal strategies where a class of transient nonrigid nanoclusters can be made globally stable using dissipative driving. The ability to design self-assembly in arbitrary far-from-equilibrium systems has the potential to lead to the bottom-up synthesis of new kinds of functional materials.

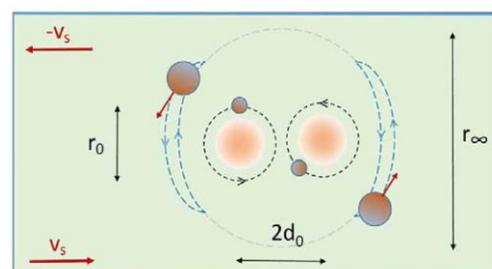
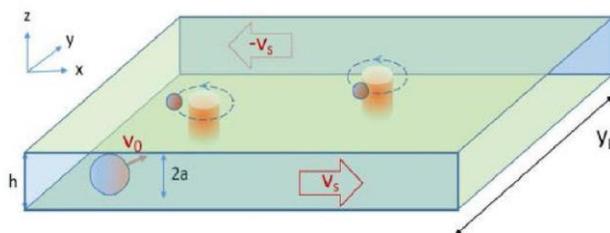
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### P1.11 Dynamics of trapped artificial microswimmers in a shear flow

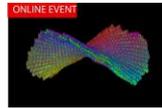
Tanwi Debnath and Pulak Ghosh

University of Calcutta, India

The motion of artificial microswimmers like self-propelled Janus particles in a suspended fluid is generally associated with backflows which vary with their self-propulsion mechanism. Janus particles are nano to micro meter sized entities having two distinct faces, only one of which is chemically or physically active. A class of Janus particles are called self-propelled Janus which can move extracting energy from surrounding by creating concentration or thermal gradient at the vicinity of their active surfaces. In course of transport process of such particles through artificial or biological channel, particles encounter various types of obstacles and thus they can be trapped. In order to overcome the trap, a detailed knowledge of the dynamics of trapped particles is necessary both in absence as well as presence of fluid flow. We numerically investigate the effect of hydrodynamic interaction of a pair of identical artificial microswimmers bound inside two harmonic traps in a thin sheared fluid film [1]. Hydrodynamic pair coupling is characterized by two-dimensional Oseen tensor which is proportional to the particle radius to film thickness ratio [2]. On increasing such ratio above a certain threshold, a transition occurs between a free regime, where each swimmer orbits in its own trap with random phase and a strong synchronization regime, where the two swimmers strongly repel each other to an average distance larger than both the trap distance and their free orbit diameter. The problem has significant applications in nano technology and biomedical sciences.



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## **P1.12 Monomer aggregation and pretransitional ordering in DNA liquid crystals**

Simone Di Leo, Giovanni Nava and Cristiano De Michele

Università degli Studi di Milano, Italy

Short DNA duplexes (6-20 base-pairs) with end-to-end attractive interactions in aqueous solution show liquid crystal nematic (N) ordering. While DNA nematics have been extensively observed and characterized, studies of pretransitional behaviour are still missing. To this end we used static light scattering technique to investigate the pre-transitional isotropic-nematic (I-N) behaviour of 12-base-long DNA duplexes with stacking interactions as a function of concentration  $I$ . We performed depolarized scattering experiments in the isotropic phase in a wide range of temperature, spanning from the no aggregation condition (high temperature) to the temperature at which I-N transition occurs.

The experimental results show a continuous increase of the depolarized scattered intensity ( $I_{dep}$ ) as the temperature is lowered. Such a  $I_{dep}$  growth is not only due by linear aggregation of duplexes (aggregation number  $M$ ), but also reveals the presence of clusters in which the duplexes are orientationally correlated, making the relationship between  $M$  and  $I_{dep}$  not trivial.

To disentangle the processes characterizing pre-transitional behavior, the  $I_{dep}$  as a function of  $T$  and  $c$  were analyzed in two steps.

Firstly, in order to free the  $I_{dep}$  from  $T$  dependencies unrelated to both aggregation process and development of orientational correlations, we normalized the data by the scattered intensities of a similar DNA duplex with not interacting ends (external mismatches).

Secondly, in order to get the information about the orientational correlations as a function of  $T$ , we performed computer simulations that allowed us to quantify how much “orientational drag” is induced on neighbouring duplexes by aggregation.

The simulation results in combination with a theoretical model allowed us to interpret the  $I_{dep}$ , obtaining  $M$  as a function of  $T$  and the stacking energy between the interacting DNA duplexes.

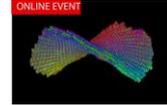
Our results give an insight about the development of local orientational order both far and in proximity of the I-N phase boundary.

## **P1.13 Self assembled colloids and their aggregation in an anisotropic solvent**

Devika Gireesan Sudha, Jocelyn Ochoa and Linda S Hirst

University of California Merced, USA

The mutual attraction between colloidal particles in an anisotropic fluid, such as the nematic liquid crystal phase can lead to the formation of hierarchical aggregate morphologies distinct from those that tend to form in isotropic fluids. Previously it has been prohibitive to study the aggregation process for a large number of colloids due to the difficulty of achieving a well dispersed initial colloid distribution. I will be talking about a recently developed self-assembling colloidal system, by our group, to investigate this process. Hollow, micron-scale colloids are formed in-situ in the nematic phase and subsequently aggregate to produce fractal structures and dense gels, the structure of which is determined by the quench depth through the isotropic to nematic phase transition. We use confocal fluorescence microscopy over a wide range of length scales to measure



aggregate structure as a function of quench depth, observed ageing mechanisms in the gels and explore the driving mechanisms for segregation in this unique system. Our analysis reveal that aggregate dynamics depend on a combination of Frank elasticity relaxation, spontaneous defect line annihilation and internal fracturing.

### **P1.14 The anomalous transport of tracers in an active bath**

Omer Granek, Yariv Kafri and Julien Tailleur

Technion, Israel

We derive the exact long-time dynamics of a tracer particle coupled to an active bath. In contrast to previous studies, we find the memory and noise correlations to possess long-time tails with exponents that depend on the tracer symmetry. For an asymmetrically shaped tracer, the tails yield superdiffusion and divergent friction. For a symmetric tracer, they yield normal diffusion and finite friction. When a symmetric tracer is small compared to the active particle run-length, the noise becomes anticorrelated at late times and the active bath-induced friction becomes negative.

### **P1.15 Underscreening in concentrated electrolytes**

Hannah Hayler, Carla Perez-Martinez, James Hallett and Susan Perkin

University of Oxford, UK

Electrolytes are ubiquitous: they are found in cells, the sea, and in technology. Our understanding of dilute electrolytes is well established as Poisson-Boltzmann electrostatics and Debye-Hückel theory are applicable. On the other hand, understanding the behaviour of concentrated electrolytes is challenging due to electrostatic correlation and steric effects.

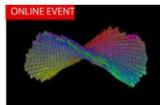
Surface force analysis has been used to measure unexpectedly long electrostatic screening lengths that appear to increase with concentration (cf. dilute electrolytes) for a variety of systems [1, 2]. This phenomenon is known as underscreening and the screening length,  $\lambda_S$ , scales according to the following empirical relationship at high ion concentration,  $c$ ,

$$\lambda_S \sim IBca^3 \quad (1)$$

where  $a$  is the ion-pair diameter and  $IB$  is the Bjerrum length [3].

We present further surface force measurements across films of deep eutectic solvent (DES) [4] and alkali metal nitrate solutions. These concentrated systems display long electrostatic screening lengths consistent with the underscreening phenomenon. We revisit underscreening in ionic liquids and consider the influence of surface curvature on the observed screening length. We also check the validity of the underscreening relationship and find that the screening length does indeed scale

with  $ca^3$  for the alkali metal nitrate and chloride solutions studied. Finally, we discuss how  $a$  should be defined for a concentrated electrolyte by considering the influence of hydration on this parameter.



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### **P1.16 Effects of hybrid lipids on the structure of a model cellular membrane of mixed lipids**

Prashant Hitaiishi, Priya Mandal and Sajal Kumar Ghosh

Shiv Nadar University, India

Plasma membrane is a semipermeable membrane that separates the interior of a biological cell from the outer environment. Phase-separated domains known as ‘rafts’ of definite size and composition control the physiological functions of the membrane. The size and thermodynamic stability of the domains depend on the electrostatic and hydrophobic interaction among the lipids used to form a model membrane [1, 2].

In the present work, we have investigated the role of hybrid lipids (HLs), which have one saturated and one unsaturated chain, in controlling the self-assembly of lipids in a model cellular membrane. Langmuir Blodgett (LB) technique on lipid monolayers formed at air-water interface and X-ray reflectivity (XRR) on supported lipid multilayers have been implemented to study the physical and structural properties of the membrane. XRR data have shown two sets of equidistant Bragg peaks of phase-separated domains in which one peak corresponds to the saturated lipid and another to unsaturated lipid. Addition of HLs has been observed to alter this phase behavior of the membrane along with reducing the phase-transition temperature of the saturated lipids. The ‘swelling method’ has been used to analyze the XRR data to obtain the electron density profile (EDP) of a membrane that has provided the quantitative information about the structural parameters of the membrane. Area-surface pressure isotherms obtained using LB system have been analyzed to calculate the in-plane elasticity and excess Gibbs free energy. Results obtained from it suggests that HLs help in mixing the saturated and unsaturated lipids in the membrane.

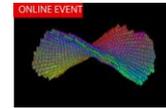
- [1] Heberle, Frederick A., and Gerald W. Feigenson. “Phase separation in lipid membranes.” Cold Spring Harbor perspectives in biology 3, no. 4 (2011): a004630.
- [2] Veatch, Sarah L., and Sarah L. Keller. “Separation of liquid phases in giant vesicles of ternary mixtures of phospholipids and cholesterol.” Biophysical journal 85, no. 5 (2003): 3074-3083.

### **P1.17 Active Surfaces and Defect-Mediated Morphogenesis**

Ludwig A Hoffmann, Livio N Carenza and Luca Giomi

Leiden University, Netherlands

There is growing evidence for the importance of topological defects in morphogenesis with several recent experiments [1-3] observing that the presence of defects fundamentally changes the morphodynamics of tissues and guides their shape changes. However, a detailed understanding and explanation of these observations is still missing.



We present an analytic theory describing the dynamics of an active surface, a two-dimensional deformable surface coupled to an active liquid crystal on the surface. We show how introducing defects can influence the dynamics of the active surface and, in particular, how a buckling-like instability can arise at the position of a defect. We supplement our analytic theory with simulations.

Our findings offer an explanation for the recent observations and are relevant to understanding morphogenesis and active surfaces in general.

- [1] Keber et al. Science 245 (2014)
- [2] Guillamat et al. BioRxiv (2020)
- [3] Maroudas-Sacks et al. Nat. Phys. 17 (2021)

### P1.18 Defect Loops in Three-Dimensional Active Nematics as Active Multipoles

Alexander Houston and Gareth Alexander

University of Warwick, UK

We develop a description of defect loops in three-dimensional active nematics based on a multipole expansion of the far-field director, with this global description complementing an earlier local analysis [1]. The multipole coefficients have interpretations in terms of the defect loop geometry, with the dipole and quadrupole terms in the director leading to active stresses that make a non-zero contribution to the total force and torque acting on the defect loop respectively. Consequently, defect loops are generically both self-motile and self-orienting, although the quadrupole coefficient is non-zero only for non-planar loops. We find that only twist-type loops possess stable force- and torque-free configurations, providing a possible explanation for their observed predominance [2]. Lastly, we determine the far-field structure of the fluid flows generated by the defect loops through derivatives of a fundamental active nematic flow response.

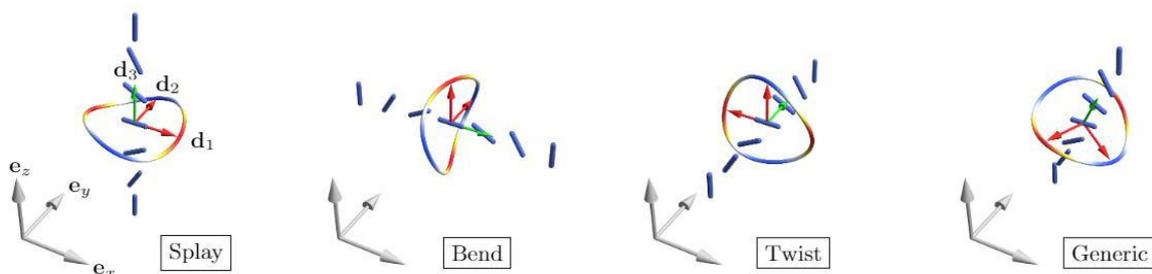


Fig. 1: Schematic illustration of defect loops, highlighting those of splay, bend and twist type. The blue rods show a cartoon of the director on a line passing through the centre of the loop. Also shown is the frame that provides a global description of the defect loop to quadrupole order - in green the  $\mathbf{d}_3$  direction which defines the dipole vector and in red the  $\mathbf{d}_1$  and  $\mathbf{d}_2$  directions which define the quadrupole tensor.

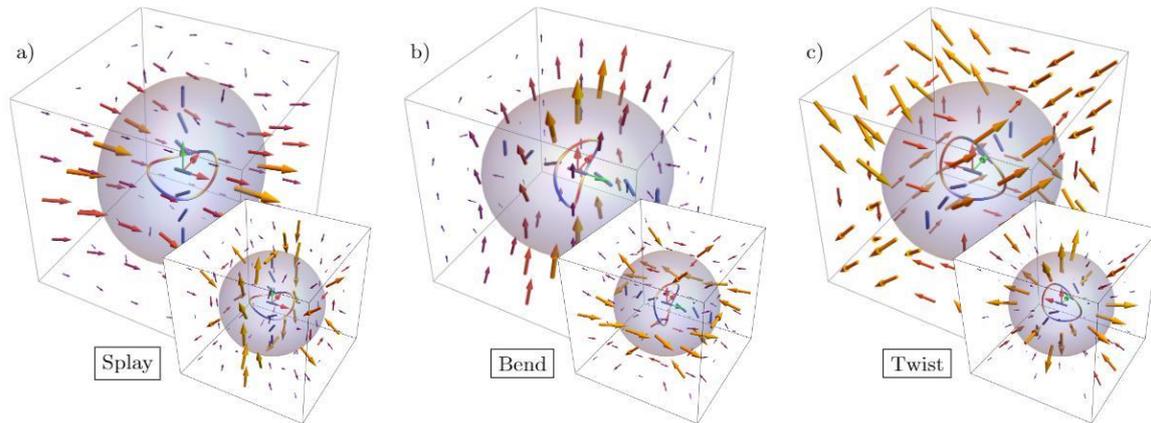
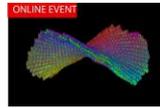


Fig. 2: The asymptotic flows induced by defect loops. Dipole contributions are shown for each type of defect loop, with the quadrupole flows shown as an insets. A) and b) show directed and rotational flows resulting from the net forces and toques acting on loops of splay and bend type – the stable twist loop in c) shows neither.

- [1] J. Binysh *et al.*, Three-dimensional active defect loops, *Phys. Rev. Lett.* **124**, 088001 (2020).
- [2] G. Duclos *et al.*, Topological structure and dynamics of three-dimensional active nematics, *Science* **367**, 1120 (2020).

### P1.19 Cells moving against obstacles: the response of a drop of active matter to external forces

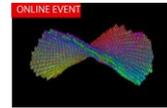
Aondoyima Ioritim-Uba, Aurore Loisy, Silke Henkes and Tanniemola Liverpool

University of Bristol, UK

So far, mathematical models of cell motility and cell migration have not fully explored the effect of external forces. These forces, either coming from cell-cell tugging or from outside the cell, are important for the functionality of cells and tissues. Experiments show that external forces can alter cell stiffness, induce migration, alter cell shape/ induce remodelling, and alter cell phenotype. Here, we model a single cell as an incompressible active nematic droplet moving on a flat rigid substrate subject to external forces at its boundaries. We work in two dimensions, where the drop is characterised by the height of its free surface above the substrate.

From force balance in the very viscous regime, we derive, and numerically solve, a differential equation for the free surface shape of the droplet. We produce a 2-D phase diagram, where the axes correspond to push or pull/squeeze by the applied forces, in which the phase boundaries are delineated by drop velocity, substrate traction, and moments of the free surface. The motion of a passive drop is clearly separated into two phases, and is symmetric in the phase plane about the pull/squeeze axis. With activity, more phases emerge, and we find that two have zero traction (between droplet and substrate) in the bulk. We also believe that the model encodes droplet breakup, which we identify by the free surface touching the substrate.

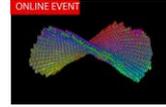
Our results show that cell shape and motile behaviour is modulated by external forces and are qualitatively in line with experimental results reported so far. The relation that we have derived between cell-substrate traction and applied force, and between cell velocity and applied force could be investigated by measuring the cell-substrate force using e.g., traction force microscopy and pushing/pulling the cell with a micropipette.

**Day 2 – Wednesday 7 July****Virtual Poster Session 2: 16:25–17:55pm**

- P2.1 **Viscosity of a solution of polyelectrolytes near the rod limit**  
Dora Izzo, Universidade Federal do Rio de Janeiro, Brazil
- P2.2 **Constructing many-body mesoscopic models of fluids from bottom-up coarse-graining**  
Jaehyeok Jin, University of Chicago, USA
- P2.3 **Separation of Active-Dipolar Cubes In Applied Fields**  
Martin Kaiser, University of Vienna, Austria
- P2.4 **Estimate locus of critical point for hard-core potential like yukawa and bukingham with using global isomorphism approach**  
Andrey Katts, I.I. Mechnikov Odessa National University, Ukraine
- P2.5 **Stability of an axisymmetric fluid column with an anisotropic interfacial layer**  
Jason Klebes, University of Leeds, UK
- P2.6 **Spatial extent of avalanches affects the yielding transition in amorphous solids**  
Daniel Korchinski, University of British Columbia, Canada
- P2.7 **Geometric and Topological Entropies of Sphere Packing**  
Jack Logan, Stony Brook University, USA
- P2.8 **Nucleation in the two dimensional Ising model in the presence of random impurities**  
Dipanjan Mandal, University of Warwick, UK
- P2.9 **Directional assembly of DNA nano-chambers into polymer-like structures**  
Deniz Mostarac, University of Vienna, Austria
- P2.10 **Magnetic nanogels in magnetic field**  
Ivan Novikau, University of Vienna, Austria
- P2.11 **Control of motility and trajectories of active droplets in a nematic environment by light**  
Mojtaba Rajabi, Kent State University, USA
- P2.12 **Ferromagnetic Nematic Phases of Charged Magnetic Nanoplatelets**  
Margaret Rosenberg, University of Vienna, Austria
- P2.13 **Shear-induced phase transition in aqueous solution of ionic liquids**  
Gunjan Sharma, Shiv Nadar University, India
- P2.14 **Thermo-orientational light action on liquid crystals with a free surface**  
Sergey Shvetsov, Lebedev Physical Institute / Lomonosov Moscow State University, Russia



- P2.15 Reversible Trapping of Colloids in Microgrooved Channels by Diffusiophoresis**  
Naval Singh, Loughborough University, UK
- P2.16 Phase behaviour of active Janus particles in three dimensions**  
Katherine Skipper, University of Bristol, UK
- P2.17 Transition to collective motion in two-dimensional microswimmer suspensions**  
Viktor Skultety, The University of Edinburgh, UK
- P2.18 Spontaneous formation of chiral domains in a flowing achiral nematic liquid crystal**  
Qing Zhang, Massachusetts Institute of Technology, USA
- P2.19 Fabrication of porous poly(methyl methacrylate) membrane for passive cooling application**  
Thành Nguyễn Tuấn, University of Science and Technology of Hanoi, Vietnam



## P2.1 Viscosity of a solution of polyelectrolytes near the rod limit

Dora Izzo

Universidade Federal do Rio de Janeiro, Brazil

We consider a solution of rodlike polyelectrolytes at low concentrations, far from the isotropic-nematic critical concentration and focus on various aspects of screening and its consequence on the system viscosity; we focus on the dependence of the viscosity on the polyelectrolyte concentration. In a charged rod, the presence of screened electrostatic interactions may induce rod bending due to a modified persistence length; as a result, the end-to-end distance becomes smaller than the contour length. In order to describe how this effect impacts on the solution viscosity, we extend the results for the viscosity of neutral rods in solution to the case of nearly stiff charged rods and obtain expressions for the viscosity in the dilute and semidilute regimes. We find a non-monotonic dependence of the reduced viscosity on the rod concentration, qualitatively similar to that of flexible modelled polyelectrolytes; the results are interpreted in terms of a competition between chain stiffening and solution screening in the different regimes of concentration. We compare our predictions with experiments and find a good qualitative agreement.

## P2.2 Constructing many-body mesoscopic models of fluids from bottom-up coarse-graining

Jaehyeok Jin

University of Chicago, USA

In the field of multiscale modelled soft condensed matter, the complex organization and transport phenomena of fluids require a mesoscopic description beyond the molecular scale. These models are often substantiated from mesoscale (fluid mechanics) and macroscale physics (statistical field theory), but their underlying microscopic foundation is not yet well-defined. This poster is designed to deliver a systematic connection between the mesoscopic model and microscopic nature using bottom-up coarse-graining methods. Based on the many-body dissipative particle dynamics and classical density functional theory, the explicit many-body conservative interaction is determined to faithfully reproduce the mesoscopic structure of fluid. The dissipative and fluctuation forces are then obtained by the proposed novel parameterization algorithm. This algorithm is built upon pairwise decomposable friction kernels under both non-Markovian and Markovian limits, where the dynamic features at the reduced resolution are nicely recapitulated. The construction of many-body dissipative particle dynamic models of fluids that can account for its microscopic nature allows for the design of bottom-up-driven mesoscopic models that naturally bridge mesoscopic and macroscopic physics. This novel approach is expected to open up a new rigorous method for constructing bottom-up multiscale models for soft condensed matter systems.



## P2.3 Separation of Active-Dipolar Cubes In Applied Fields

Martin Kaiser and Sofia Kantorovich

University of Vienna, Austria

The term "active matter" describes a class of out-of-equilibrium systems, whose ability to transform environmental energy to kinetic energy is sought after in multiple fields of science. A challenge that still remains is the creation of nanometer sized active particles, whose motion can be effectively directed by externally applied stimuli. Adding a magnetic component and therefore being able to direct the motion of active nanoparticles with an applied magnetic field proved promising and effective in previous experimental and theoretical studies. However, magnetic, steric and active interactions in suspension of those particles lead to unexpected properties of the systems that have yet to be discussed before developing reliable applications. In the present study, we employ molecular dynamics simulations to shed light on the internal mechanisms taking place in suspension of magneto-active nanometer sized particles in an applied constant magnetic field. We show that the orientation of the dipole compared to the active force acting on the particles determines the direction of the swimming motion while a magnetic field is applied. Particles with different orientations therefore separate under the influence of a magnetic field. However, this is only the case in dilute systems where interparticle interactions are mitigated by the low concentrations of particles. In dense systems, those interactions overpower the sorting effect and the bulk of particles perform a swimming motion in the same direction. We elucidate the underlying internal mechanisms of this effect by directing the separate components of the interparticle interactions and their influence on this behaviour.

## P2.4 Estimate locus of critical point for hard-core potential like yukawa and bukingham with using global isomorphism approach

Andrey Katts

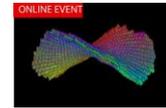
I.I. Mechnikov Odessa National University, Ukraine

We discuss possibility application projective form of global isomorphism approach [1,2] for Hard core Yukawa potential (HCYF) and Buckingham potential. Both of them have hard core, but their attractive parts are different.

$$\Phi_Y(r) = \begin{cases} \infty, & r < \sigma \\ -\varepsilon \cdot \frac{\exp(-\gamma(r - \sigma))}{r}, & r \geq \sigma \end{cases} \quad \Phi_B(r) = \begin{cases} \infty, & r < \sigma \\ -\frac{\varepsilon}{1 - \frac{6}{a}} \cdot \frac{6}{a} \left( \exp(-a(r - \sigma)) - \frac{C}{r^2} \right), & r \geq \sigma \end{cases}$$

Projective form of approach allows to explain disappearing stable liquid phase [3] in case too short-range Yukawa potential. We estimate value of parameter , in which liquid branch is not exist. We conclude that native form of global isomorphism between real liquid and lattice gas doesn't work for metastable phase of liquid.

Fig. Depending limit density of parameter , which shows applicability of approach to HCYF if .



Using the scale properties of potential allows to find locus of critical point for this potential without applying molecular dynamic.

Fig. Parametric function . Green and red points are data of [4] and blue line is theoretical function.

- [1] Kulinskii, V. L., Phys. Chem. B, 141, 054503 (2010)
- [2] Bulavin, L.A. and Kulinskii, V.L. Chem. Phys., 133, 134101 (2010)
- [3] Hagen M. H. J., Frenkel D. Chem. Phys - 1994. - T. 101. - №. 5. - C. 4093-4097.
- [4] P Orea, C Tapia-Medina., Chem. Phys., 132, 114108 (2010)

## P2.5 Stability of an axisymmetric fluid column with an anisotropic interfacial layer

Jason Klebes

University of Leeds, UK

A large class of fluid-fluid interfaces, such as lipid membranes or those in particle-stabilized (Pickering) emulsions, are defined by an interfacial layer of molecules or particles. Characteristics such as local lipid composition or particle density influence stability and morphology of interfaces, while being themselves influenced by surface geometry. As a model for a characteristic of an interfacial layer with phase behavior and geometric interactions, we examine so-called n-atic orientational order. This order parameter represents correlations in, for example, the (1-atic) vector direction of the tilt of lipid molecules, orientation of a nematic liquid crystal layer, or orientation of a hexatic arrangement of particles.

We examine a sinusoidally modulated cylindrical interface which, in addition to having the usual surface tension and bending rigidity, is coupled to the orientational order parameter field representing a surface layer. Breakup or stability of cylinder-like fluid threads is of interest in emulsion formation and aging. Similar interface shapes are also seen in metastable sheared emulsions and as vesicles.

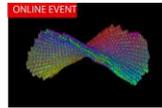
Stability of the interface and configurations of the field are evaluated analytically and via a Markov chain Monte Carlo lattice simulation of the order parameter field coupled to surface geometry. We find that an ordered surface layer has a stabilizing effect on the system, providing additional resistance to deformation. Where curved surface shapes nevertheless dominate, we see a spatially differentiated state where orientational order is destroyed locally on certain splay-inducing regions. On the given topology, field morphology depends crucially on the order of the interfacial layer's discrete rotational symmetry ( $n=1$  or  $6$ ). While at low orders we merely see orientational order suppressed to varying degrees, for hexatic surface layers, which are highly sensitive to distortion, distinct patterns of rotations and defects emerge in response to curvature.

## P2.6 Spatial extent of avalanches affects the yielding transition in amorphous solids

Daniel Korchinski, Celine Ruscher and Joerg Rottler

University of British Columbia, Canada

Amorphous solids are a disparate class of materials defined by their lack of long-range crystalline order, and includes examples with fundamental constituents in the range of millimeters (e.g.



bubble-rafts) to nanometers (metallic glasses). Despite the breadth of this class, the yielding transition in these materials shows signs of a universal phase transition in the statistics of slip events, particularly for systems in the athermal quasistatic driving regime. The residual stress distribution,  $p(x)$ , describes the proximity to yielding for mesoscopic regions of the amorphous solid. Since the weakest region in the system governs overall stability,  $p(x)$  affects the statistical properties of macroscopic failure events known as avalanches, by governing how much strain energy can be accumulated before failure. In the thermodynamic limit,  $p(x)$  has a pseudogap of the form  $p(x) \sim x^\theta$ . Using a mesoscopic model of amorphous plasticity under strain-controlled athermal quasistatic loading conditions, we show that for finite-systems  $p(x)$  has a previously unrecognized intermediate power-law deviating from the main  $\theta$  exponent, before entering a terminal plateau with  $p(x \ll 1) \sim L^{-p}$ . By studying the residual stress distribution immediately after avalanches of different sizes, we show that the smallest and largest avalanches introduce two characteristic scales to  $p(x)$ . These scales affect the distribution of residual stress in the system, coupling the avalanche size distribution to the residual stress distribution in a new way. This alters the established scaling relations for the yielding transition in amorphous solids and therefore alters the yielding exponents.

## P2.7 Geometric and Topological Entropies of Sphere Packing

Jack Logan and Alexei Tkachenko

Stony Brook University, USA

We present a statistical mechanical description of randomly packed spherical particles, where the average coordination number is treated as a macroscopic thermodynamic variable. The overall packing entropy is shown to have two contributions: geometric, reflecting statistical weights of individual configurations, and topological, which corresponds to the number of topologically distinct states. Both of them are computed in the thermodynamic limit for isostatic packings in 2D and 3D, and the result is further expanded to the case of “floppy” particle clusters. The theory is directly applicable to sticky colloids, and in addition, generalizes concepts of granular and glassy configurational entropies for the case of non-jammed systems.

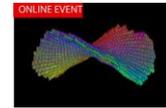
## P2.8 Nucleation in the two dimensional Ising model in the presence of random impurities

Dipanjan Mandal and David Quigley

University of Warwick, UK

Nucleation phenomena are ubiquitous in nature. The study of nucleation with changing parameters, e.g., temperature, pressure, field, applied shear, etc., has diverse industrial applications. Modelling nucleation from the solution is an active area of research with relevance to pharmaceutical manufacture, biomineral formation and other highly complex precipitation processes. In every real and experimental system the presence of impurities is unavoidable, and yet numerical studies of nucleation are nearly always conducted for entirely pure systems.

We study nucleation from a metastable phase to the stable phase in the two dimensional Ising model on square lattice in the presence random “spin-0” impurities. We consider both static and dynamic impurities. We show that the nucleation rate decreases with increasing the impurity density for the static case. To calculate the nucleation free energy as a function of the cluster size, we use an Umbrella Sampling method with biased infinite square well potential. Fitting the free



energy plot with the Becker Doring expression of the Classical Nucleation Theory, we show that the interfacial free energy per unit length decreases linearly with increasing impurity density at different temperatures. In a previous study Ryu and Cai [Phys. Rev. E 82, 011603 (2010)] have shown the agreement of the nucleation rates obtained from the Becker Doring theory and from simulations using Forward Flux Sampling. We also show that the same observation is true for the system with random static impurities when the impurity density is low. Both the critical nucleus size and the barrier height decrease monotonically with increasing impurity density. In the case of dynamic impurities, we observe the preferential occupancy of the impurities at the boundary positions of the nucleus when the temperature is low. This further boosts enhancement of the nucleation rate due to lowering of the effective interfacial free energy.

## P2.9 Directional assembly of DNA nano-chambers into polymer-like structures

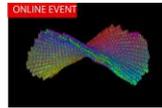
Deniz Mostarac, Yan Xiong, Pedro A. Sanchez, Oleg Gang and Sofia Kantorovich

University of Vienna, Austria

Construction of smart materials with sophisticated magnetic response by incorporating magnetic nanoparticles within permanently cross-linked structures (i.e. magnetic filaments), opens up the possibility for synthesis of more complex, highly magneto-responsive systems.[1,2] Recent advances, advocating an assembly mechanism where the structure building instructions are embedded into nanoparticles via DNA origami frames, finally open the door towards synthesis of such materials with tuneable magnetic response mechanical properties. It has been shown that a pre-defined set of different DNA-framed nanoparticles, along with DNA polyhedral frames, enable designing diverse planar constructs, 1D, 2D and 3D frameworks. [3,4] Although it is well understood that sophisticated hierarchical structures could be assembled by modulating the dimensionality, specificity and strength of connections between with DNA polyhedral building blocks, other intrinsic properties of connections are not explored. Some tunable properties are highly relevant to morphologies of large-scale organizations, and mechanical properties of the larger superstructures they form.

Using a combination of experiments and molecular dynamics computer simulations, we present how tunable properties, namely the length and arrangement of DNA linkers of DNA nano-chamber polyhedral frames reflects itself on morphologies of large-scale organizations. More specifically we demonstrate that by tuning the aforementioned properties, one can achieve assembly into polymer-like, linear nanofiber structures. We use computer simulations to predict polymer equilibrium properties of the arising structures for a broad range of lengths and rigidities, elucidating the impact of the monomer shape.

- [1] Sánchez, P. A., et al. *Macromolecules* 48.20 (2015): 7658-7669.
- [2] Mostarac, D., et al. *Nanoscale* (2020).
- [3] Liu, W., et al. *Nature chemistry* 8.9 (2016): 867.
- [4] Tian, Y., et al. *Nature materials* 15.6 (2016): 654.



## P2.10 Magnetic nanogels in magnetic field

Ivan Novikau, Sofia Kantorovich and Pedro Sanchez

University of Vienna, Austria

Nanogels (NGs) with multifunctionalized magnetic nanoparticles (MNPs) have demonstrated the ability to effectively destroy cancer cells *in vivo*, without causing visible damage to healthy organs [1]. The presence of MNPs inside the NGs also offers an additional mechanism to control their properties by means of applied magnetic fields.

Our study of a suspension of NGs loaded with MNPs in zero-field case showed that the structural properties of a single gel, and the self-assembly in the given system, strongly depend on the strength of the dipole-dipole interaction (dipolar coupling parameter) between the MNPs [2].

Here, we investigate a suspension of magnetic NGs in a constant external magnetic field by means of molecular dynamics computer simulations [3]. Each NG is initially modelled as a system of bead-spring polymer chains randomly cross-linked into a polymer network. MNPs are arbitrary incorporated into this network.

We find that even weak fields lead to drastic changes in the structure factors of both, the embedded MNPs and of whole NGs. But what is even more curious, is that the polymer matrix of nanogels enhances the magnetization of free MNPs.

[1] Qing Wu et al., Nat. Commun., 10 (240), 2019.

[2] Novikau et al., JMMM, 498, 2020.

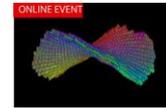
[3] Novikau et al., J. Mol. Liq., 307, 2020.

## P2.11 Control of motility and trajectories of active droplets in a nematic environment by light

Mojtaba Rajabi, Hao Wang, Hend Baza and Oleg Lavrentovich

Kent State University, USA

One major objective of active matter science is to create controllable machines capable of transforming out-of-equilibrium dynamics into useful work. Active colloids are seen as candidates for this role. Recently, active droplets of a suspension of bacteria were found capable of rectifying their interior chaotic flows into a directional self-locomotion when placed in a nematic environment [1]. Here, we demonstrate control over the direction and speed of active drop's propulsion using light. The droplets distort the director of the nematic environment and form either a point defect of dipolar symmetry or an equatorial disclination loop of quadrupolar symmetry around themselves. The droplets of dipolar symmetry propel with the point defect leading the way while the droplets of quadrupolar symmetry are stationary. A laser beam pointed to the vicinity of the droplet can transform the director configuration to the desired symmetry and thus affect the motility and polarity of propulsion. When the laser is pointed to one side of a droplet of quadrupolar symmetry, it melts the nematic there. Once the laser is switched off, the nematic recovers and forms a point defect that causes propulsion in the direction of the defect. The opposite transformation from the dipolar to the quadrupolar configuration is achieved by melting the nematic everywhere in the



drop's vicinity using the beam. When the laser is switched off, a disclination ring is formed and the droplet stops. Focusing the beam on the opposite side of the droplet forms the point defect there and reverses the polarity of motion. The tuning of the motility and propulsion direction of active droplets represents a step forward in the development of controllable microswimmers.

The work is supported by the NSF grant DMR-1905053.

Rajabi M, Baza H, Turiv T, Lavrentovich OD, Directional self-locomotion of active droplets enabled by nematic environment. *Nature Physics*,(2021).17:260-266.

## P2.12 Ferromagnetic Nematic Phases of Charged Magnetic Nanoplatelets

Margaret Rosenberg and Sofia S. Kantorovich

University of Vienna, Austria

In recent decades, advances in synthesis techniques have opened up a new subfield in the study of magnetic soft matter: the study of anisotropic and anisometric magnetic colloidal suspensions. The persistent interest in investigating and refining anisotropic colloidal systems comes from the knowledge that colloidal anisometry can be used as an effective control parameter to tune both self-assembly scenarios and thermodynamic, rheological and phase behavior of dipolar (magnetic) soft matter[1]. For instance, it is now possible to synthesize discotic mesogens with a dipole moment perpendicular to the long axis of the particle. This combination of anisotropy and anisometry results in a suspension which can form a macroscopic ferromagnetic nematic phase at room temperature[2].

While the phase behavior of hard platelets is already well-known, the influence of the added dipole moments, platelet size polydispersity and electrostatic repulsion on the isotropic to nematic phase transition are not yet fully understood. Bringing together experimental investigations of the suspensions, theoretical predictions and simulations, we aim to characterise the phase behavior of such systems in detail. This contribution will focus on the computational work, recreating the system through Molecular Dynamics simulations in different approximations (raspberry and Gay-Berne), then studying the influence of parameters such as the dipole moment or aspect ratio on the phase transition, as well as analysing the structural properties of the system in different phases.

[1] P. Tierno, *Phys. Chem. Chem. Phys.*, 16, 23515-23528 (2014)

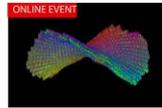
[2] A. Mertelj, D. Lisjak et al, *Nature*, 504, 237-241 (2013)

## P2.13 Shear-induced phase transition in aqueous solution of ionic liquids

Gunjan Sharma, Saheli Mitra and Sajal Kr Ghosh

Shiv Nadar University, India

An ionic liquid (IL) is a salt in liquid state below 100°C, consisting of a cation and an anion, one of which possesses an organic component. Because of the non-volatile property, these solvents have a high recovery, and hence they are considered environment friendly green solvents. It is necessary to study the detailed physicochemical properties of IIs for designing and processing techniques and find suitable operating conditions for IL-based systems. In the present work, flow behavior of



aqueous solutions of an IL is investigated. Dynamic viscosity measurements indicate a non-Newtonian shear thickening in the solutions. Polarizing optical microscopy (POM) shows the pristine samples to be isotropic which display optical texture under the shear. This suggests a shear induced change in the underlying structure of the self-assembled mesoscopic aggregates.

Moreover, differential scanning calorimetry (DSC) measurements confirm the change of shear thickened liquid crystalline phase to an isotropic phase upon heating. The detailed structural information of various mesoscopic aggregates before and after the shear is obtained by small-angle X-ray scattering (SAXS) measurements. These measurements suggest the existence of optically isotropic cubic phase before shear which gets distorted after the shear. This work provides the detailed structural evolution of mesoscopic aggregates of the IL in aqueous solution and corresponding viscoelastic property of the solution.

## **P2.14 Thermo-orientational light action on liquid crystals with a free surface**

Sergey Shvetsov, Alexander Zolot'ko, Gleb Voronin, Alexander Emelyanenko, Pavel Statsenko and Sergey Trashkeev

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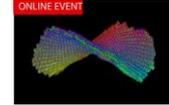
The film of a nematic liquid crystal with a free surface (LCFS) is an unusual optical system, the nonlinear optical response of which is determined by various orientational processes and also by the distortion of surface shape.

The air environment hinders heat outflow at even a weak light absorption by the liquid crystal substrate and the liquid crystal is locally heated. This leads to the occurrence of thermally induced processes. As for isotropic liquids, a reduction in the surface tension with an increase in temperature causes a curvature of the surface shape and a decrease in the thickness of the liquid crystal layer in the illuminated area, which results in the self-defocusing of light beam.

Another process is the light-induced orientation caused by the temperature gradients (thermal orientational effect). The heat outflow in the bulk of the LCFS leads to an axially symmetric director reorientation with an axis normal to the substrate plane, forming the umbilical defect. The thermal orientational effect occurs at light beam intensities one order of magnitude lower than the threshold of the light-induced Fredericksz transition. Unlike most of the light-induced orientational phenomena, this effect does not depend on the polarization and angle of incidence of the light beam. The thermal orientational effect of the light beam is strongly non-local: the area of the orientation deformation can be several times larger than the diameter of the light beam.

The obtained results open up new possibilities in the development of highly sensitive optical materials based on LCFS, and also indicate the importance of taking into account the thermally induced processes when considering the interaction of light beams with soft matter.

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## P2.15 Reversible Trapping of Colloids in Microgrooved Channels by Diffusiophoresis

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In recent years, an increasing interest in harnessing chemical energy in the form of solute concentration gradient has led to the exploration of colloidal particle manipulation by diffusiophoresis (DP) in microfluidic devices [1]. Transient salt concentration gradients have been successfully used to achieve enhanced particle transport into dead-end structures by DP and diffusioosmosis (DO) effects [2-3]. In this study, we report a novel mechanism for reversible trapping of particles in dead-end micro-structures via steady-state solute gradients in a continuous flow setting [4]. A microchannel, made of optical adhesive glue, was fabricated by photo-/soft-lithography techniques and fitted with a transverse microgrooved wall. The charged fluorescent colloidal particles were accumulated within the microgrooves by pumping parallel electrolyte solutions into the device junction. The spatial distribution of particles within the channel was characterized via confocal microscopy and a numerical investigation was carried using finite element simulations. As shown by the confocal scans in the figure, we found that particles accumulate within the flow recirculation region beneath the groove entrance due to a combination of DP transport and hydrodynamic effects. The trapping phenomenon is fully reversible and particles can be cyclically trapped into and released from the grooves by controlling the salt concentration of the parallel streams via a flow switching valve. The proposed method offers great potential for microfluidic bio-analytical testing applications, including bio-particle pre-concentration and signal amplification.

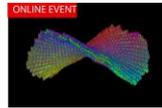
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## P2.16 Phase behaviour of active Janus particles in three dimensions

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We present an experimental study of the phase behaviour of active Janus particles in a three-dimensional system. Janus particles are an experimental realization of so called ‘active Brownian’ motion, a simple model where the rotational diffusion of particles driven with constant velocity produces activity. Janus particles are characterized by a silica or polystyrene core with a metal cap, such that the two hemispheres have distinct dielectric properties. In an AC electric field, the polarisation of the two hemispheres produces unbalanced ionic flows which ‘tug’ at the particle, propelling it forwards. [1].



Sedimentation has generally confined the study of Janus particles to quasi two-dimensional systems. Gravitational effects can be reduced with small diameter particles, and whilst the activity remains two-dimensional the system can access three dimensional structures.

The purpose of this work is to study the full phase diagram of Janus particles in three dimensions. The frequency and strength of the field as well as the ionic concentration of the solvent all contribute to a rich and complex catalogue of behaviours. The experimental data will be compared with molecular dynamics simulations of dipolar active particles to identify the driving forces of the collective behaviour.

If active systems are to be used in the design of functional materials, an understanding of their phase behaviour is paramount. Additionally, the study of active matter in three dimensions has implications in Biology; polar active gels of protein filaments form the cytoskeletons of cells, with the contraction of these gels producing cell movement [2].

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## **P2.17 Transition to collective motion in two-dimensional microswimmer suspensions**

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A collection of microswimmers immersed in an incompressible fluid is characterised by strong orientational interactions due to the long-range nature of the hydrodynamic fields generated by individual organisms. As a result, suspensions of 'pusher' swimmers exhibit a state often referred to as collective motion or 'bacterial turbulence', which is dominated by jets and vortices compromising many microswimmers. The onset of collective motion can be understood within a mean-field kinetic theory for dipolar swimmers. In 3D, the theory predicts that the instability sets in at the largest scale available to the suspension.

Here, we present a mean-field kinetic theory for a dilute suspension of run-and-tumble dipolar swimmers confined to a 2D plane embedded in a 3D fluid. We analyse the stability of the homogeneous and isotropic state and find two types of instability: one is the analogue of the orientational instability in 3D systems, while the other is associated with strong density variations absent in 3D. In contrast to 3D suspensions, both instabilities can occur at the smallest possible scale, and we discuss their implications for the ensuing collective motion.



## **P2.18 Spontaneous formation of chiral domains in a flowing achiral nematic liquid crystal**

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An achiral nematic fluid in a microfluidic cell could be expected to form achiral structures in a pressure-driven flow. Surprisingly, we find the spontaneous emergence of chiral structures when an achiral lyotropic chromonic liquid crystal (LCLC) in the nematic phase relaxes from a high velocity flow to a steady-state lower velocity flow. The chirality results from a periodic double-twist deformation of the liquid crystal and leads to striking stripe patterns vertical to the flow direction. We demonstrate that this occurrence of chiral structures can be rationalized by the disparate elastic constants of the LCLC; the peculiarly low twist elastic constant compared to the bend and splay elastic constants of LCLCs allows for twist deformations, which lead to spontaneous symmetry breaking. We show that the wavelength of the periodic structures depends on the local flow velocity, which is set by the competition between the elastic torque and viscous torque acting on the chiral structures.

## **P2.19 Fabrication of porous poly(methyl methacrylate) membrane for passive cooling application**

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Passive cooling is a green cooling solution in climate crisis. The material transfer heat from the ambient to the universe via thermal radiation with wavelength in the atmospheric's transparent window 8-13 $\mu$ m. Poly(methyl methacrylate) (PMMA) is a material well suited for such purpose, with rich vibrational modes in this range. In cooperation with porous structure, fabricated by phase inversion method, PMMA membrane could achieve a sizable cooling effect. We study the radiative cooling of PMMA thin film when cast on glass substrate. Our films show proper optical results with promising temperature reduction. Passive cooling is a green cooling solution in climate crisis. The material transfer heat from the ambient to the universe via thermal radiation with wavelength in the atmospheric's transparent window 8-13 $\mu$ m. Poly(methyl methacrylate) (PMMA) is a material well suited for such purpose, with rich vibrational modes in this range. In cooperation with porous structure, fabricated by phase inversion method, PMMA membrane could achieve a sizable cooling effect. We study the radiative cooling of PMMA thin film when cast on glass substrate. Our films show proper optical results with promising temperature reduction.

