"The Physics of Evolving Matter: Memory, Learning and Evolution"
The Geilo School 2022, March 21-31, Geilo, Norway

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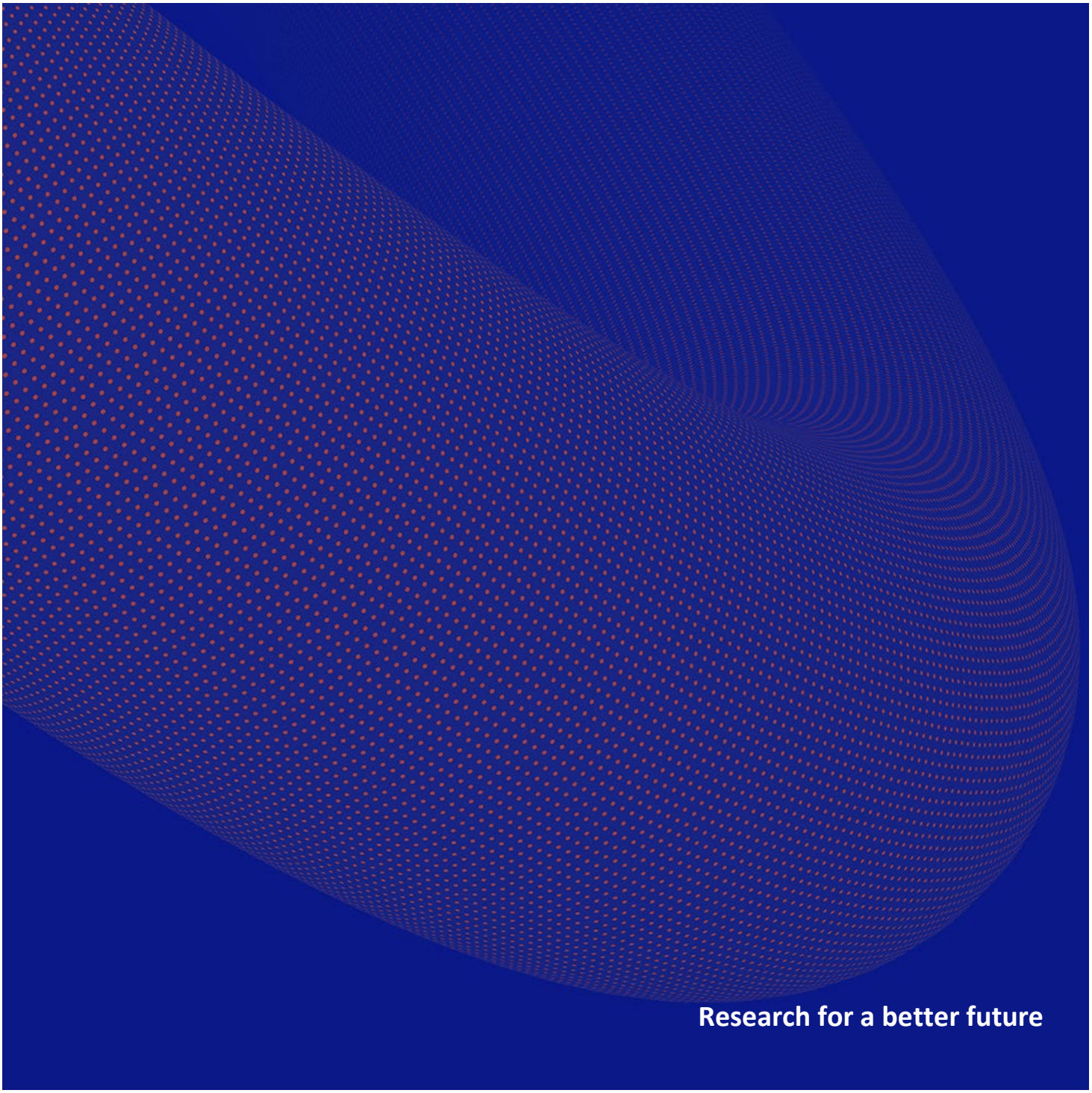

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Title:
"The Physics of Evolving Matter: Memory, Learning and Evolution",

The Geilo School 2022, March 21-31, Geilo, Norway

Summary:
This report contains the complete program, poster abstracts, lists of lecturers and participants at the “Geilo School” held at Bardøla hotel, Geilo (Norway) March 21-31, 2022.

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Contents

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1 Introduction

This report contains the complete program, poster abstracts, lists of lecturers and participants at the "Geilo School" (GS) held at Bardøla hotel, Geilo (Norway) March 21-31, 2022. This is the twenty-sixth GS in a series held every two years since 1971 [1]. The theme of the school was "The Physics of Evolving Matter: Memory, Learning and Evolution", which is in the forefront of current research in soft matter science, complex matter physics, and biological physics. Condensed Matter Physics involves the study and characterization of how individual components like atoms, molecules, particles, and other entities self-organize is some collective state and where the behavior of the collective is more important than the behavior of the individuals. The physics of evolving matter has applications in biology.

The sub-themes of the School are outlined below.

A) *Memory* formation in matter, as an interdisciplinary theme, is situated at the crossroads of physics, biology, chemistry, and computer science. It relates to the ability to encode, access, and erase traces of history in the state of an evolving system.

B) *Learning* - Modern machine learning technology offers a new arena for study and characterization of how individual components self-organize is some collective state in condensed matter.

C) *Evolution* is traditionally understood as the change in the heritable characteristics of biological populations over successive generations. It could also be denoted fundamental physical processes that give rise to biological phenomena. Condensed matter physics concepts might provide a useful perspective in evolutionary biology and animate matter.

Financial support to this Geilo School was principally from the Research Council of Norway, grant no. 333233. Support was also received from the EU H2020-MSCA-ITN-ETN project "PICKFOOD" (Pickering emulsions for food applications) - grant agreement number 956248, Norwegian University of Science and Technology (NTNU), Trondheim (Norway), and the Institute for Energy Technology, Kjeller (Norway).

A list of previous Geilo schools may be found here:
https://ife.no/en/project/the-geilo-schools/

May 2022

Arne T. Skjeltorp

Director of the Geilo School 2022

2 Program of the Geilo School 2022

The Physics of Evolving Matter: Memory, Learning and Evolution

1st Day Monday March 21		
Arrival Bardøla 19:00		*Chartered bus Oslo to Bardøla hotel, Geilo*
19:00-19:15	*Registration*	
19:30	*Welcome Drink in the Bar*	
20:00	*Dinner*	
22:00	Arne Skjeltorp	OPENING of the Geilo School 2022 in "Bardølasalen"
2nd Day Tuesday March 22		
08:30-10:30	Matthieu Wyart	Analogies between the theory of deep learning and granular materials
10:30-11:30	Giovanni Volpe	Machine learning and active matter
11:30-15:30	*Discussions, activities, lunch*	
15:30-17:30	Giovanni Volpe	Machine learning and active matter (ctd.)
17:30-18:30		Tutorial group meetings with lecturers of the day
3rd Day Wednesday March 23		
08:30-11:30	Jean-François Joanny	Microscopic and macroscopic descriptions of tissues
11:30-15:30	*Discussions, activities, lunch*	
15:30-17:30	**Poster session 1**	
17:30-18:30		Tutorial group meetings with lecturers of the day
4th Day Thursday March 24		
08:30-11:30	Amy Rowat	-Cells as materials: principles in mechanobiology in health and disease -Harnessing knowledge of cells as materials for sustainable protein production
11:30-15:30	*Discussions, activities, lunch*	
15:30-16:30	Matthieu Wyart	Allostery and protein evolution
16:30-17:30	Irep Gozen	Seminar
17:30-18:30		Tutorial group meetings with lecturers of the day
5th Day Friday March 25		
08:30-11:30	Eric Clement	Exploration and transport of motile bacteria in complex environments
11:30-15:30	*Discussions, activities, lunch*	
15:30-17:30	**Poster session 2**	
17:30-18:30		Tutorial group meetings with lecturer of the day
6th Day Saturday March 26		
08:30-11:30	Jasna Brujic	- The encoding of a sequence to fold into the structure of proteins - Droplet swimmers that leave a trail behind them
11:30-15:30	*Discussions, activities, lunch*	
15:30-17:30	Marta Zlatic Albert Cardona	Key features of a reinforcement learning circuit in the insect brain
17:30-18:30		Tutorial group meetings with lecturers of the day
7th Day Sunday March 27		
Free	***Choice of excursions to nearby scenic places or various skiing or hiking events in the mountains***	***Depends on weather***

8th Day Monday March 28		
08:30-09:30	Marta Zlatic Albert Cardona	Key features of a reinforcement learning circuit in the insect brain (Ctd.)
09:30-11:30	Patrick Tabeling	What the writing of a microfluidic book helps to learn
11:30-15:30	*Discussions, activities, lunch*	
15:30-17:30	Olli Ikkala	Triggerable memory and materials responses algorithmically inspired by biological learning
17:30-18:30		Tutorial group meetings with lecturers of the day
9th Day Tuesday March 29		
08:30-09:30	Olli Ikkala	Triggerable memory and materials responses algorithmically inspired by biological learning (Ctd.)
09:30-11:30	Julia Yeomans	Active Matter: Applications in Mechanobiology
11:30-15:30	*Discussions, activities, lunch*	
15:30-16:30	Julia Yeomans	Active Matter: Applications in Mechanobiology (Ctd.)
16:30-17:30	Françoise Brochard-Wyart	Micropipette aspiration of proteins coated bubbles: role of compressibility and porosity
17:30-18:30		Tutorial group meetings with lecturers of the day
10th Day Wednesday March 30		
08:30-09:30 09:30-10:30 10:30-11:30	Pawel Pieranski	- Nucleation, collisions and rewiring of disclinations - Nucleation and collisions of monopoles in the Dowser Texture - Strain-induced emission of folded dislocation loops in cholesterics
11:30-15:30	*Discussions, activities, lunch*	
15:30-17:30	Maria Helena Godinho	Cellulose animate colorful patterns
17:30-18:30		Tutorial group meetings with lecturers of the day
19:30	***Geilo School Banquet Dinner***	***Geilo School 50th year jubilee. Geilo awards, Poster Prizes etc.***
11th Day Thursday March 31		
Departure 08:30		*Chartered bus Geilo to Oslo*

Sponsors:

3 Poster Abstracts

In-Vivo monitoring of Peripheral Nerve Regeneration using SESORS molecules.

Namrah Azmi, Abhishekh Tiwari, Atul Chaskar
National Centre for Nanoscience and Nanotechnology, University of Mumbai, India

Abstract:

Using Spatially Offset Surface Enhanced Raman Spectroscopic Molecules/ SESORS Molecules for Real-time imaging of peripheral nerve regeneration.

Fabrication of nanofiber scaffolds consisting of aligned inner surface of PLGA fibers for directional guidance for promoting the sciatic nerve regeneration was carried out. PLGA conduit with aligned fibers provided strong orientation guidance and exhibit desirable degradation 12 weeks post-implantation.

Further, Gold nanoparticles (GNPs) seem to enhance cell proliferation along with biomolecule attachment and act as SERS (Surface Enhanced Raman Spectroscopic) molecule. The objective of introducing Metal-based nanostructures (MNSs) into PLGA substrates is to impart other biological functions, such as stimulation of regeneration by means of incorporating metallic elements with therapeutical effects. Even at low concentrations, MNSs are capable of inducing surface morphological changes within the polymer matrix.

Many reports indicated that GNPs are nontoxic, and GNPs of diameter 30 and 50 nm have been shown to be “blood compatible” and did not induce any detectable platelet aggregation, immune response, or change in plasma coagulation time. The synthesized Au nanoflowers are ideal SERS substrates because of the abundance of “hot” spots generated by their special surface topography which could result in substantial local electromagnetic field enhancement.

Soy protein isolate (SPI), an abundant low-cost plant protein with excellent hydrophilicity, biocompatibility and tailor able biodegradability can be used as a blending component to improve mechanical properties and bioactivity of material. SPI improves tensile strength, surface wettability, cytocompatibility and in vivo degradability (12 weeks). At 20-40% ratio, SPI promotes neural cell extension and differentiation in vivo. On combination with PLGA it increases cell identification signals and help dissolve GNPs for functionalization.

Surface enhanced spatially-offset Raman spectroscopy (SESORS) offers a non-invasive, or minimally invasive, technique for detection of neurotransmitters through the skull, which is non-destructive and signal can be obtained in 2 minutes or less. Therefore, a Raman spectrum comprising several different ‘‘Raman lines’’ generated by scattering from different molecular vibrations provides a vibrational ‘‘fingerprint’’ of a molecule. Raman imaging is thus highly sensitive and specific with precise chemical structure identification and penetration to individual nodes of Ranvier.

Optimizing processing of plant derived Pickering food emulsions.

Namrah Azmi – Stayfit Nutrisupplies
Dr. Leonard Rweyemamu – Stayfit Nutrisupplies
Prof. Jon Otto Fossum – NTNU (Norwegian University of Science and Technology)

Abstract:

Pickering emulsions based on food-grade oil and edible nanoparticles extracted from Moringa Oleifera tree.

Extensive food wastage all over the world has resulted in enormous impact on environment. Food wastage is caused as a result of chemical deterioration of food such as oxidation of lipid, vitamins and other constituents of food. Thus many such foods are stabilized by surfactants. Standard surfactants have been widely used till now due to their properties such as easy use, low cost and relative control. But the need of reduction of volatile organic compounds and carbon footprints are been possessed as a threat for surfactants industrial use. Therefore, use of Pickering particles to produce physically stable emulsions and improving oxidative stability of emulsions can be a solution to surfactants. Pickering emulsions are emulsions stabilized by solid-particles, which generally provide a more stable system than traditional surfactants.

Pickering particles can reside at the interface of droplets and bubbles, consequently providing them, resistance against fusion (coalescence) and coarsening (Ostwald ripening) meaning that the droplets and foams become physically stable. Pickering emulsions have good biocompatibility and can be used as carrier for the delivery of bioactive compounds. While the basic principle of stabilizing emulsions with Pickering particles seems simple, stabilization of complex foods is a significant and complicated physical problem, and limited information is currently available for food systems. Therefore, there is a need to develop new food grade Pickering particles.

Hence, our project aims to develop novel Pickering emulsions for Food Applications using solid organic particulate materials as stabilizers which generally include edible substances such as polysaccharide, protein or lipid particles. Solid particles under consideration in our case would be Moringa seed cake protein, Moringa leaf protein or modified Moringa seed cake/ leaf protein. Emulsion formation and stability using selected Moringa extracts will be investigated under various conditions such as imposed flow.

The project will therefore provide a structure with unconventional strategies to study and develop Pickering emulsions and to assess their applications in safe, healthy and functional foods. Attaining this objective depends on our physical comprehension of emulsion stability and processing, preparation of food-grade Pickering particles along with is characterization utilizing highly advanced methods unconventional in food science.

Memory formation in adaptive networks

Komal Bhattacharyya[1], David Zwicker[1], Karen Alim[1,2]

[1] Max Planck Institute for Dynamics and Self-organisation, Germany
[2] Physics Department, Technical Universität München, Germany

Abstract:
Continuous adaptation of networks like our vasculature ensures optimal network performance when challenged with changing loads. Here, we show that adaptation dynamics allow a network to memorize the position of an applied load within its network morphology. We identify that the irreversible dynamics of vanishing network links encode memory. Our analytical theory successfully predicts the role of all system parameters during memory formation, including parameter values which prevent memory formation. We thus provide an analytically tractable theory of memory formation in disordered systems.

Confinement effects on the phase transitions of the polymer nanotubes and nanowires

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[1]École Centrale de Lyon,
[2]Université Claude Bernard Lyon 1, CNRS, UMR 5223

Abstract

Polymer nanostructures are broadly used in the scientific fields, i.e., organic electronics, energy harvesting, sensing, etc. Confinement effects that are caused by the nanoscale processing of polymers can lead to a behavior that is different from the bulk. Here the effects of confinement on the phase transitions of P(VDF-TrFE) nanowires and nanotubes with varying thicknesses are reported.

In this thesis, the state-of-the-art of the polymer-based nanomaterials was reviewed. The main objective of the study is to understand how physical properties are changing in the nanoconfinement.

Using broadband dielectric spectroscopy (BDS), differential scanning calorimetry (DSC), X-ray diffraction (XRD), change in the physical properties was investigated. Transmission electron microscopy (TEM) was used to study the morphology of the P(VDF-TrFE) samples. Crystallization temperature decreases with stronger confinement, with the new crystallization temperature peaks arising for nanotubes. Melting temperature and the Curie transition are not affected by nanoconfinement. New relaxation effect was measured by BDS, with the nature of this effect supposedly being orientation effects caused by nanoconfinement.

Results imply that nanoconfinement enhances affects the phase transitions of nanowires and nanotubes, which could potentially enhance other electrical and dielectric properties of polymer materials, comparing with bulk, therefore giving the possibility to improve material properties.

Rupture of thin films subjected to thermal fluctuations and shear

Vira Dhaliwal, Christian Pedersen, Andreas Carlson:

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Thin fluid films commonly occur in soft matter and biological systems. When a thin liquid film rests between a solid substrate and a gas phase, it may spontaneously rupture due to attractive van der Waals forces between the interfaces. We model this physical system using the lubrication approximation and study the influence of a shear stress at the upper interface along with thermal fluctuations that are relevant on a nanometric scale. Finite-element simulations demonstrate that an external shear stress can indeed suppress the rupture of unstable surface perturbations. Thermal fluctuations, meanwhile, render the thin film unstable by triggering long-wavelength perturbations. Increasing the strength of thermal fluctuations decreases the time required for rupture to occur. Beyond the initial growth of an instability, van der Waals forces become dominant, and thermal fluctuations and shear seem not to play a major role.

Capturing the emergence of hydrophobin protein amyloid function

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Secreted ubiquitously by filamentous fungi, hydrophobins (HFBs) are a family of proteins that tailor the surrounding environment to a particular lifestyle by modifying the physicochemical properties of interfaces via self-assembly into amyloid and amyloid-like structures. In this poster I will describe the remarkable sequence diversity of this protein family and the methods that I have developed with my collaborators to explain the evolution, synthesis, and function of these proteins that defy the currently held views built on protein science's central structure-function paradigm. My work suggests the intriguing possibility functional amyloid assembly in the HFB family is driven by non-hierarchal assembly processes within the complex and dynamic ecosystem of the fungus' surroundings. It is this environment that both regulates and directs functional assembly and so the properties of the environment are central to explanations of hydrophobin protein function. As such, I argue that hydrophobins can serve as a model protein family to integrate our understanding of material assembly, ecology, biology, and protein science. This line of investigation will lead to improving our understanding and ability to harness the function, as well as dysfunction, of amyloid structures across length scales.

Memory in mechanical metamaterials under cyclical shear deformations

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We designed a cylindrical metamaterial using a network of nonuniform beams that exhibits novel mechanical properties under shear deformations such as a programmable Poynting effect and oscillatory shear and normal responses. By applying a pre-compression, the vertical beams experience a double-well potential and transfer to a left-buckled or a right-buckled state. The bistable local beams perform as hysteric elements (hysterons) that can change their state when the system is under different boundary conditions and deformations. The general state of the system is determined by a sequence of hysterons states, which depend on the deformation pathway and can change through shearing the system. These transitions can be complex and irreversible, leading to a tunable state setting in the system that is functional as a memory unit. Understanding the governing principles in state transitions of such hysteric systems provides an insight into the designing and information processing in complex materials.

Conductive micropaths made from assembled 1D particle structure: novel method of fabrication, and micropath characterization

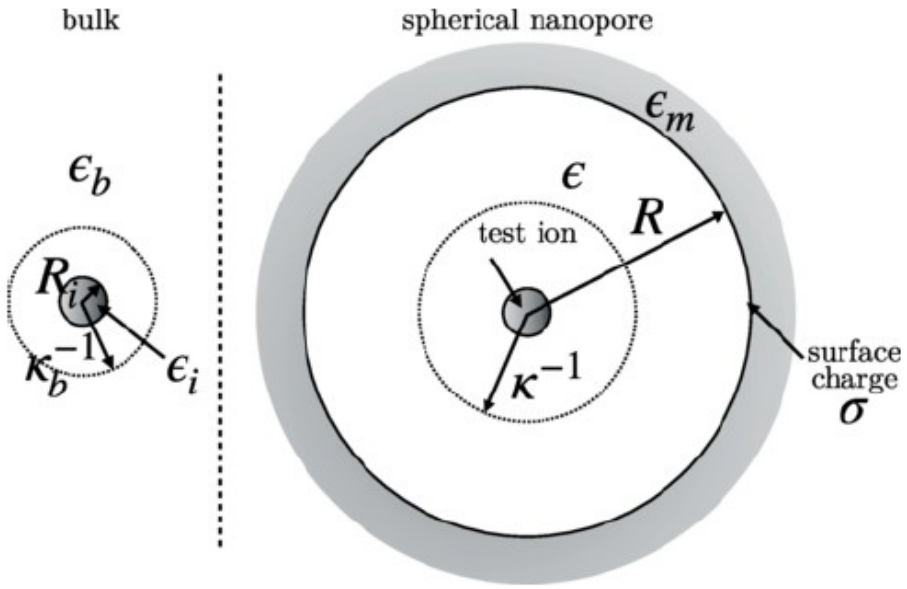
Yaroslav Harkavyi,[1] Konrad Giżyński,[2] Zbigniew Rozynek[1,3]

[1] Faculty of Physics, Adam Mickiewicz University, Poznań, Poland
[2] Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland
[3] CADENAS, Poznań, Poland

Assembly of single-particle thick one-dimensional microstructures on substrates is desired for performing different fundamental studies, and holds promise for a variety of practical applications. This includes electronic applications, i.e., formation of highly conductive electrical paths. There are many approaches for fabrication of such structures, but they are expensive, time-consuming, or inefficient, requiring access to advanced tools and laboratories. Here we report a method that overcomes these limitations and facilitates the continuous production of particle paths outside bulk liquid on various substrate materials and morphologies, using a variety of particle materials with wide size range. The method is simple yet robust and easy to implement, and is straightforwardly scalable, involving a synergetic action of electric-field assembly, capillary and electrostatic interactions. Using our developed method, we have fabricated micropaths of different widths, height-to-width ratio, and the magnitude of electrical conductivity. The postprocessed particle structures can be used in electronic applications, for example, as conductive micropaths.

Competition between Born solvation, dielectric exclusion, and Coulomb attraction in spherical nanopores

Théo Hennequin



The recent measurement of a very low dielectric constant, ε, of water confined in nanometric slit pores leads us to reconsider the physical basis of ion partitioning into nanopores. For confined ions in chemical equilibrium with a bulk of dielectric constant $\varepsilon_b > \varepsilon$, three physical mechanisms, at the origin of ion exclusion in nanopores,are expected to be modified due to this dielectric mismatch: dielectric exclusion at the water-pore interface the solvation energy related to the difference in Debye-Hückel screening parameters in the pore, κ, and in the bulk κ_b, and the classical Born solvation self-energy. Our goal is to clarify the interplay between these three mechanisms and investigate the role played by the Born contribution in ionic liquid-vapor (LV) phase separation in confined geometries. We first compute analytically the potential of mean force (PMF) of an ion of radius R_i located at the center of a nanometric spherical pore of radius R. Computing the variational grand potential for a solution of confined ions, we then deduce the partition coefficients of ions in the pore versus R and the bulk electrolyte concentration ρ_b. We show how the ionic LV transition, directly induced by the abrupt change of the dielectric contribution of the PMF with κ, is favored by the Born self-energy and explore the decrease of the concentration in the pore with ε both in the vapor and liquid states. Phase diagrams are established for various parameter values and we show that a signature of this phase transition can be detected by monitoring the total osmotic pressure as a function of R. For charged nanopores, these exclusion effects compete with the electrostatic attraction that imposes the entry of counterions into the pore to enforce electroneutrality. This study will therefore help in deciphering the respective roles of the Born self-energy and dielectric mismatch in experiments and simulations of ionic transport through nanopores.

Article : https://doi.org/10.1103/PhysRevE.104.044601

ACOUSTIC MANIPULATION OF PARTICLES AND BIOLOGICAL CELLS

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Acoustic manipulation of micro-objects (particles, cells, bacteria) can be achieved by using ultrasonic standing waves in a fluidic or microfluidic resonator [1,3], as illustrated in Fig 1. In an acoustic resonator, by matching the proper geometrical and physical parameters the acoustic radiation force (ARF) can gather particles at the pressure nodal plane. There, particles are in levitation an equilibrium position where the radial component of the ARF allows their aggregation creating one or several aggregates. When particles are close of each other, another force, the Secondary Bjerknes force [4,5] start to act keeping them close together and leading a stable aggregate.

Here we show several applications of the acoustic levitation and the collective behavior of different species under acoustic radiation force: bacteria, metallic nanorods and Mesenchymal stem cells. The three examples concern active matter.

Nevertheless, janus nano rdos in water are not active as in hydrogen peroxide. But we discover that nanorod under acoustic radiation force are self-propelled, we called that effect: self-acoustophoresis.

Active flows in endoplasmic reticulum networks

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The endoplasmic reticulum (ER) is a network of fluid-filled tubules and sheets which performs essential cellular functions such as protein and lipid synthesis and processing. Single particle tracking in peripheral ER networks has revealed slow diffusive motion inside nodes (i.e. the junctions between tubules) and much faster transport across tubules (Holcman et al. (2018) "Single particle trajectories reveal active endoplasmic reticulum luminal flow", *Nature Cell Biol.* **20**: 1118). The uncoordinated stochastic pinching of tubules was proposed as a possible mechanism behind ER solute transport. We study theoretically the fluid dynamics of such active networks using a viscous hydraulic model of realistic ER geometries forced stochastically by finite-size pinching. Our model predicts that the tubule-pinching mechanism results in weak but wildly fluctuating flows that only slightly enhance the effective diffusivity of transported particles so that solute transport remains dominantly diffusive. The predicted traversal speeds are an order of magnitude lower than those measured experimentally, suggesting that the pinching hypothesis is not able to account for ER solute transport. The pinch parameters may be pushed to recover the high speeds seen in experiments, but they are associated with unrealistic rates of pinching and pinch sizes. We further investigate the possibilities of the contractions of tubular junctions or peripheral ER sheets as driving mechanisms; junctions are again too weak as generators of flow, and peripheral ER sheets introduce spatial inhomogeneities not observed in experiments. Our study therefore does not support pinching-driven flows as the origin of the measured active ER flow and the biological mechanism behind active solute transport in the ER still remains to be identified.

Phase field modelling of active interacting cells that grow and divide

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A multiphase field model is used to study growth of a colony of cells such that the cell shape is captured at a high resolution. The model includes exponential growth and division of cells. Contact inhibition of proliferation is included to allow only the cells in the periphery of the colony to grow. It is observed in the model that the colony radius grows linearly, and it's shape is isotropic for non migrating cells and anisotropic for migrating cells. The model also includes a novel interaction which allows for adhesion between cells. This can be used to achieve various geometries of packing confinement using a cell colony.

Designing kinetic features of self-assembly

Ella M. King, Carl P. Goodrich, Chrisy Xiyu Du, Sam S. Schoenholz, Ekin D. Cubuk,
Michael P. Brenner
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Abstract: Self-assembly research to date has yielded incredible control over the design and assembly of complex static structures. However, biological systems rely not just on control over structures, but also control over dynamics. For instance, embryonic development relies on precisely tuning relative rates of tissue growth. In order to design synthetic materials that parallel the complexity of biological systems, we need to gain control over dynamical features in addition to structural ones. Here, we demonstrate the ability to design two canonical kinetic features in self-assembly systems, crystallization rates and transition rates, by building on advances in automatic differentiation. We further discuss current efforts in the inverse design of nucleation seeds whose structures can tune the rate of crystal formation.

Using Neutron Spin Echo Spectroscopy to Probe Lipid Membrane Dynamics and How they are Affected by Antimicrobial Peptides.

Vladimir Koynarev[a], Josefine Eilsø Nielsen [a], Ingo Hoffmann[b], Reidar Lund[a]

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[b]Institute Laue Langevin (ILL), Grenoble, France,

Abstract

In recent years increasing scientific efforts have been made towards understanding the dynamics of lipid bilayers at different length and timescales, from the motion of individual lipids to large scale dynamics of cellular membranes. It is largely believed that membrane dynamics have a significant impact on the overall properties of the membrane, and that they are influenced by both the membrane composition and external additives, such as proteins or nanoparticles[1]. The experimental study of membrane dynamics, in particular thickness and bending fluctuations which happen at an intermediate length and timescale, has only recently become viable through the use of Neutron Spin Echo (NSE) spectroscopy[1,2].

Here we aim to investigate how the presence of antimicrobial peptides (AMPs) affect the bending and thickness fluctuation in phospholipid liposomes as model membranes using NSE. This is done as an effort towards further elucidating the antimicrobial activity of these peptides. Initial NSE experiments with DMPC containing liposomes show that the membrane stiffness changes upon addition of the AMP, Indolicidin. By correlating the dynamics data from NSE with structural small-angle X-ray/neutron scattering (SAXS/SANS) data[3], we aim to obtain insight into how the AMPs affect and compromise bacterial membranes.

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2. Woodka, A. C., Butler, P. D., Porcar, L., Farago, B., & Nagao, M. (2012). Lipid Bilayers and Membrane Dynamics: Insight into Thickness Fluctuations. In Physical Review Letters (Vol. 109, Issue 5). American Physical Society (APS). https://doi.org/10.1103/physrevlett.109.058102
3. Nielsen, J. E., Bjørnestad, V. A., Pipich, V., Jenssen, H., & Lund, R. (2021). Beyond structural models for the mode of action: How natural antimicrobial peptides affect lipid transport. In Journal of Colloid and Interface Science (Vol. 582, pp. 793–802). Elsevier BV. https://doi.org/10.1016/j.jcis.2020.08.094

QUASI-TWO-DIMENSIONAL PSEUDO-SESSILE DROPLETS CONFINED BETWEEN WETTING SURFACES

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Sessile droplets have definite shapes that are determined by surface tension, gravity, and contact angle. Droplets with extremely large contact angles can be achieved by microfabricated low-energy surfaces and by thin vapor layers that separates droplets from their underlying substrate known as the Leidenfrost effect with interesting properties. Here we show that it is possible to create stationary and moving quasi-two-dimensional pseudo-sessile droplets and that their shape corresponds to 3D sessile droplets with 180° contact angle. As with sessile 3D droplets, quasi-two-dimensional droplet thickness is restricted by capillary length, and they adopt a spherical shape when effective gravity is zero. Furthermore, quasi-two-dimensional droplets can slide with velocity that is determined by contact line drag. Our results comprise a theoretical model for drops in non-conventional dimensions, and the realization of this model in experimental work that includes static and dynamic quasi-two-dimensional droplets. Using this framework, liquid shapes, sizes and motions could be better predicted in microfluidic channels or other confined vertical systems where droplets meet edges.

Rechargeable self-assembled droplet microswimmers driven by surface phase transitions

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Swimming microorganisms and engineered artificial swimmers use multiple strategies to achieve propulsion in the viscosity-dominated microworld. A number of them use long, filamentous appendages called cilia or flagella. The motion of these slender objects is governed by a complex interplay between the driving forces, the elastic properties of the fibres, and the resistance forces of fluid.

A recently studied artificial system involving an emulsion of microscopic droplets of oil with surfactant in water exhibits swimming induced by the extrusion of elastic fibres by the droplets [1]. The extrusion is controlled by a surface phase transition of the surfactant, and it drives the motion of droplets. The transition is driven by small changes in the temperature of the environment, and can be reversed by switching between cooling and heating the system. The formation of a plastic phase by the surfactant induces shape changes of the droplets, where polyhedral shapes become energetically favourable. Further reconfiguration driven by the phase transition leads to the formation of filamentous structures originating at vertices of the now polygonal droplets. The extruded fibres undergo dynamic buckling and produce complex shapes, but also exert a force and torque on the droplets, resulting in translation and rotation of the droplets. We propose an elastohydrodynamic model for this phenomenon and describe the motion by a combination of theoretical considerations and numerical simulations. Our model serves as the basis for interpretation of experimental data and quantitatively grasps the swimming dynamics.

[1] D. Cholakova, M. Lisicki, S.K. Smoukov, S. Tcholakova, E. Lin, J. Chen, G. De Canio, E. Lauga, N. Denkov, Rechargeable self-assembled droplet microswimmers driven by surface phase transitions, Nature Physics **17**, 1050 (2021).

Directed colloidal assembly and learning with DNA reinforcement strands

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Our ability to form self-assembled materials or micro-structures currently depends on our ability to understand and form the specific interactions needed to produce a given self-assembled shape. While there has been a large amount of effort put into the development of novel techniques to create directional interactions, they remain limited both by experimental synthesis and by the fact that the required interactions must be predicted beforehand. To overcome these limitations, I'm working to develop a novel method to create self-assembled colloidal clusters without the complicated synthesis of functionalized patchy particles. By drawing inspiration from reinforcement learning algorithms, I plan to train an experimental system of DNA-labeled colloidal particles, physically reinforcing desired bonds with additional DNA strands in solution when the system moves closer to the final configuration. The system then continues to rearrange, exploring many potential configurations and receiving additional reinforcement, until the desired structure becomes the favored configuration. From an initially isotropic system, we then achieve directional interactions which favor a particle structure through experimental reinforcement learning.

Bright, Non-Iridescent Structural Coloration from Clay Mineral Nanosheet Suspensions

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Structural colors are vivid colors that originate by constructive interference following reflection and scattering from periodic structures with length scales in the range of visible light. Biological structural coloration is found in animals such as birds, marine animals, some mammalian species, and insects, as well as in certain plants. One factor of importance for natural structural coloration, as well as for their potential industrial applications, is the degree of iridescence. Bright and non-iridescent structural colorations are highly desirable, but they were limited to a handful of materials that could hardly be called sustainable. Here we demonstrate that bright non-iridescence structural coloration easily and rapidly can be achieved from suspended two-dimensional clay nanosheets. We show that brightness is enormously improved by using double clay nanosheets, thus optimizing the clay refractive index that otherwise hampers structural coloration from such systems. The non-iridescence structural colors can be precisely and reproducibly controlled from varying interlayer distances by clay concentration and ionic strength independently. Embedding such clay designed nanosheets in recyclable solid matrices could provide tunable vivid coloration and mechanical strength and stability at the same time, thus opening a new venue for the sustainable penetration of structural coloration to everyday life.

2D Magnetic Janus Clay Nanosheets

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Abstract:

2D nanosheets are of high interest for various applications, such as for those relying on encapsulation of droplets or particles, capture of molecules or liquid crystalline organization. Of particular importance are 2D nanosheets that respond to, and can be manipulated by applied magnetic fields, thus enabling extractions or aiding nematic self-organization. Here we report the successful and efficient approach of decorating inert 2D nanosheets in liquid phase with magnetic nanoparticles on one side. We use functionalized iron oxide nanoparticles and high-aspect ratio sheets of insulating transparent synthetic sodium fluorohectorite clay. Efficiency of the process is confirmed by several complementary characterization methods, including X-ray diffraction (SAXS/WAXS), spectroscopy (FTIR, UV-VIS), and microscopy techniques (SEM and AFM). Furthermore, options of tuning particle density on the nanosheets are demonstrated and possible applications will be discussed.

Unmodified Clay Nanosheets at the Air-Water Interface

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Quasi-2D nanolayers, such as graphene oxide or clay layers adhere to gas-liquid or liquid-liquid interfaces. Particularly clays are of wide general interest in this context because of their extensive and crucial use as Pickering emulsion stabilizers, as well as for their ability to provide colloidosome capsules. So far clays could only be localized at oil-water or air-saline-water interfaces in aggregated state, while our results now show that clay nanosheets without any modification can be located at air-deionized-water interfaces. The clay mineral used in the present work is synthetic fluorohectorite with a very high aspect ratio, superior quality in homogeneity and charge distribution compared to other clay minerals. This clay mineral is more suitable for achieving unmodified clay anchoring to fluid interfaces compared to other clay minerals used in previous works. In this context, we studied clay nanosheet organization at the air-water interface by combining different experimental methods: Langmuir-Blodgett Trough studies, Scanning Electron Microscopy (SEM) studies of film deposits, Grazing Incidence X-ray Off Specular Scattering (GIXOS) and Brewster Angle Microscopy (BAM). Clay films formed at the air-water interface could be transferred to solid substrates by the Langmuir-Schaefer method. The BAM results indicate a dynamic equilibrium between clay sheets on the interface and in the subphase. Because of this dynamic equilibrium, the Langmuir monolayer surface pressure does not change significantly when pure clay sheets are spread on the liquid surface. However also GIXOS results confirm that there are clay nanosheets on the air-water interface. In addition, we find that clay sheets modified by a branched polymer are much more likely to be confined to the interface.

Superconductivity in living organisms

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Superconductivity in living organisms, specifically in central nervous system and brain, was suggested as early as in 1972 by E. Halperin and A. Wolf [1]. Even before that, in 1964, W. Little developed theoretical model for room-temperature superconductivity (RTS) in organic chains of molecules linked to specific molecular complexes, which could be present in living organisms [2]. The purpose of possible RTS was first not understood. Neither were experimental evidences present showing its existence.

Situation changed when it became clear that superconductivity is efficient in quantum computing. Currently, functional superconductor-based quantum computers became reality. An opportunity appeared to explain extraordinary power of brain and nervous system. Experiments started too, first with crude electrical transport measurements of brain slices [3], then using more sophisticated nanometre-scale magnetic force microscopy [4]. The latter was intended to check ideal diamagnetism in brain nano-structures. A conclusion was made that superconductivity is likely to reside in microtubules: highly ordered quasi one-dimensional nanometre-size structures somewhat reminding those suggested by W. Little [2]. The estimate of critical temperature in brain tissue was made [3], and it was found to be close to that predicted by W. Little [2]. A concept of based-on-superconductivity quantum processing of information in living organisms was put forward [5].

In this work, new experimental evidences of RTS are given extending abilities of magnetic force microscopy to measuring cross-sections of microtubules.

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Investigating swelling and delaminating clay nanolayers in a controlled manner

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It is important to understand and control the process of swelling and delamination of nanolayered materials for many different applications, e.g. molecule or nanoparticle capture and transport or even to create structural colors [1-3]. Here we present results of experiments using particles of fluorohectorite synthetic clay ($Na_{0.5}[Mg_{2.5}Li_{0.5}]\langle Si_4\rangle O_{10}F_2$) ranging from 100 to 300 µm lateral size in saline solutions (Sodium Chloride) from 1 to 0.025 M as well as Ultra Small Angle X-ray Scattering (USAXS at CoSAXS beamline, Max IV, Lund, Sweden) to investigate nematic suspensions of this high aspect ratio (≈ 20000 [4]) clay at various salt and clay concentrations.

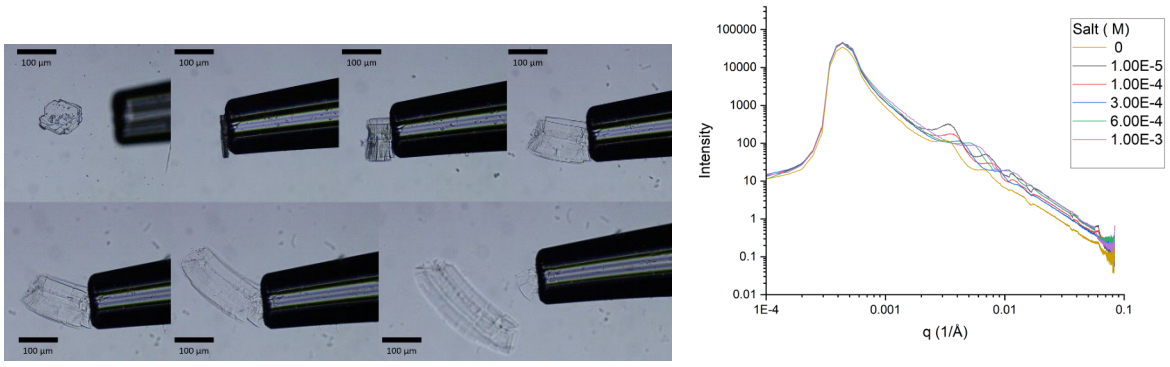

Figure 1 – (Left)Clay particle swelling with the reduction of salinity. (right)SAXS plot showing clay compacting behavior with increment of salinity.

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Graphene Confined in Layered Silicate

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The real use of graphene in electronic devices, such as field-effect transistors (FET), meets several principal complications. Opening of graphene band gap usually leads to significant drop of electron mobility; limitation of Klein tunneling paradox can prevent graphene-based devices from switching into the OFF state. Some of the complications can be overcome by combining graphene with insulating layers in two-dimensional heterostructures that allow for fabrication of a graphene-based FET with a high ON and OFF switching ratio[1] , and precise control over graphene doping. However, fabrication of such heterostructures is not trivial. The best performing heterostructures are made by manual assembly, which is not very efficient method for their mass production. We have prepared two-dimensional heterostructures more efficiently, by growing graphene from a nitrogen-carbon precursor inside the confined space of a layered silicate. This approach promises simultaneous band-gap opening in graphene and formation of final heterostructures in one step. The resulting structure has the form of a multi-layered sandwich composed of nitrogen-doped (N-doped) graphene-like layers and the single layer sheets of synthetic layered silicate, sodium fluorohectorite. Can such a large-scale production method generate well-defined and homogeneous clean system useable for FET or other electronic applications of graphene? To answer this question, we need to examine the layered heterostructure itself, to reveal the nature of the N-doped graphene-like layers. As the initial point, it is of high benefit to know how are the nitrogen atoms distributed within the graphene lattice. Electronic transport properties of sandwich multi-layers, which are important parameters for device performance, can be then explained in the context of geometry of individual layers. Nitrogen doping of graphene is the efficient way of band-gap modification, as it allows band-gap opening and its transformation to an n or a p-type semiconductor[2] .

Nitrogen can be incorporated into the graphene lattice in three different configurations[2,3,] with planar sp2 (pyridinic and pyrrolic) and tetrahedral sp3 (quaternary N) hybridizations. Depending on the level of the sp2-N doping and the geometry of the N-doped graphene lattice, band gap can vary from 0.14 eV up to 0.7 eV4. Characteristic C-C, N-C and N-N bond lengths depend on the lattice configuration and differ from the un-doped graphene[2,4]. Growth of the N-doped graphene in confined space[3] is a promising method superior to the other preparation strategies, as it provides selective formation of pyridinic and pyrrolic groups in the graphene lattice and suppress formation of quaternary N. Carbon lattice doped with planar N-sites can serve as useful building block for use in the supercapacitors, batteries, transistors, fuel cells and other semiconductor applications[2] , and also possess high activity in the oxidation reduction reactions[3] in contrast to the lattice containing quaternary N. In all cases, types of nitrogen doping, lattice geometry and defects together with the lattice distortions significantly alter both properties, performance and the suitable application potential of the N-doped graphene[2]. Its combination with layered silicate is a promising step towards the real applications.

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Olfactory navigation: how to make decisions using a broken signal

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Foraging mammals often pause to sniff in the air preceded by rearing on their hind legs or raising their head. Interestingly, this behavior emerges spontaneously during olfactory search in presence of airflow, suggesting that alternation may serve an important role during turbulent plume-tracking. To test this hypothesis, we combine fully-resolved numerical simulations of turbulent odor transport and Bellman optimization methods for decision-making under partial observability (POMDP). We show that an agent trained to minimize search time in a realistic odor plume exhibits extensive alternation together with the characteristic cast-and-surge behavior commonly observed in flying insects. Alternation is tightly linked with casting and occurs more frequently when the agent is far downwind of the source, where the likelihood of detecting airborne cues is higher relative to cues close to the ground. Casting and alternation emerge as complementary tools for effective exploration when cues are sparse. Fluid dynamics explains the alternating behavior, in fact when the environment is turbulent odor cues travel faster and further in the air than at the ground were they are slowed down by the boundary layer. We develop a model based on marginal value theory to capture the interplay between casting, surging and alternation. More generally, we show how multiple sensorimotor modalities can be fruitfully integrated during complex goal-directed behavior.

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Flow around topological defects in active nematic films

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The hydrodynamics of active nematics is characterized by an active turbulence regime whereby topological defects proliferate and interact with each other. The nematic state corresponds to orientational order, which is punctuated by half integer disclinations, as lowest energy defects. We study the flow induced by the active stress around isolated $\pm 1/2$ defects in an active nematic film in the presence of both viscous dissipation (η) and friction with the substrate (Γ). The interplay between the two dissipation mechanisms gives rise to a length scale $\ell_d^2 = \eta/\Gamma$, which sets the scale of the self-propulsion velocity for the $+1/2$ defect, and the scale for the decay of flow velocity and vorticity. Spanning vortices with alternating vorticity are formed around the defect in an active nematic film confined to a disk. The shape of these vortices, in addition to the self-propulsion of the positive defect, is determined by the relation between the discs radius R and ℓ_d. For small systems, in units of ℓ_d, the velocity is proportional to the radius. As the size become larger the velocity become set by the dissipation length and the vortices become elongated. In the limit of $R \to \infty$ the vortices closes at infinity.

SELF-ASSEMBLING OF NOVEL IONIC LIQUID CRYSTALS-BASED ON SUBSTITUTED PYRIDINIUM CATIONS

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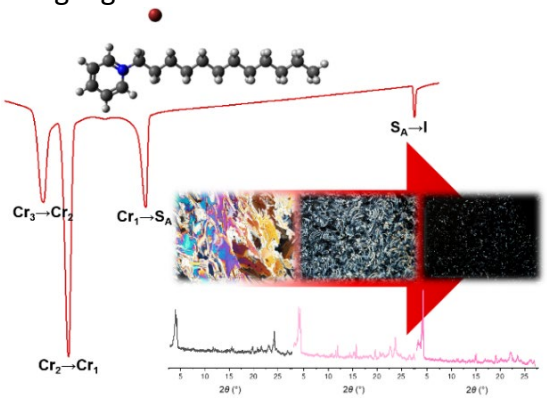
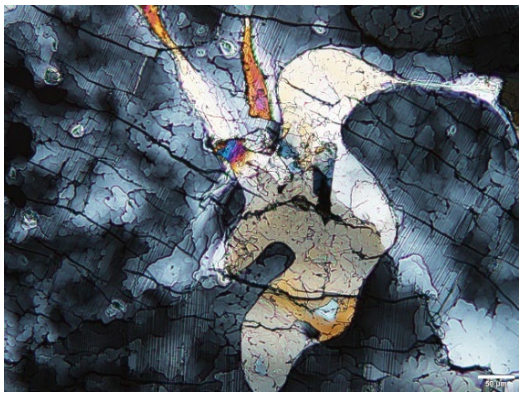
Ionic liquid crystals are soft ordered materials containing cations and anions. As they combine characteristics of both liquid crystals and ionic liquids, it is possible to tune their physicochemical and self-assembling properties by selecting specific moieties, allowing the design of new functional materials, as active pharmaceutical ingredients [1]. In this work, several pyridinium bromide derivatives were synthesized based on pyridinium and 2-, 3- or 4-methylpyridinium cations substituted with a dodecyl chain, [C_{12}-*n*-Pic][Br]. It is known that the rigidity of the cation linked to the flexibility of the alkyl moiety are main requirements for the formation of ionic liquid crystals [2]. In order to evaluate the effect of the alkyl chain length, [C_6-2-Pic][Br] and [C_{16}-2-Pic][Br] were also prepared. Microwave-assisted reactions, as a sustainable approach, were performed to reduce the reaction time, the solvent usage and to improve their yields. All compounds were characterized by spectroscopic techniques (^{1}H and ^{13}C-NMR; ATR-FTIR), Differential Scanning Calorimetry, Polarized Optical Microscopy and X-Ray Powder Diffraction. The results obtained indicate the formation of thermally induced smectic phases. The insertion of a methyl group in *meta* and *para* positions of the pyridinium ring significantly reduces the clearing point and the liquid crystalline range, when compared with the parent [C_{12}Pyr][Br] and the *ortho*-substituted. Moreover, [C_n-2-Pic][Br] (*n* = 6, 12 and 16) were further investigated by Dielectric Relaxation Spectroscopy. Lyotropic aqueous solutions are also highlighted.





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Transport among protocells via tunneling nanotubes

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We employ model protocell networks for evaluation of molecular transport through lipid nanotubes as potential means of communication among primitive cells on the early Earth. Network formation is initiated by deposition of lipid reservoirs onto a SiO_2 surface in an aqueous environment. These reservoirs autonomously develop into surface-adhered protocells interconnected via lipid nanotubes while encapsulating solutes from the ambient buffer. We observe the uptake of DNA and RNA, and their diffusive transport between the lipid compartments via the interconnecting nanotubes. By means of an analytical model we determine key physical parameters affecting the transport, such as nanotube diameter and compartment size. We conclude that nanotube-mediated transport could have been a possible pathway of communication between primitive cells on the early Earth, circumventing the necessity for crossing the membrane barrier. We suggest this transport as a feasible means of RNA and DNA exchange under primitive prebiotic conditions, possibly facilitating early replication.

Structural investigation of the gelation dynamics of colloidal silica

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Silica gels have a multitude of different applications in different areas such as drug encapsulation, matrix for production of metallic nanoparticles, fillers in cosmetic products and in oil recovery for plugging of high permeability zones. Colloidal sodium-silicates consist of anionic SiO_2 particles and Na_2O dissolved in water. As the electrolyte content of the solution is increased, for instance by adding salts (e.g. NaCl), the particle repulsion is screened and binding among the particles occur, causing gelation. The gelation is also influenced by other factors, such as temperature, solid content, divalent ion concentration and shear. In this project we investigate the structuring of colloidal silica using Small Angle X-ray Scattering (SAXS) during gelation under different conditions. In addition to this, microcapsules carrying the gelling activator will be utilized. This will allow for the initiation of the gelling to be postponed until a triggering condition is applied, achieving more control over the gelation process.

Design of SiC Nanoparticle Systems Using MD Simulation and Machine Learning

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Abstract:

We examine mechanical properties of a faceted silicon carbide system using molecular dynamics simulations and machine learning. Silicon carbide nanoparticles have in simulations been observed to transform into a faceted shape. Here, a porous system is studied, where the voids are in the shape of a faceted nanoparticle. The mechanical strength of these systems are studied as a function of the spatial locations of the inclusions. A machine learning model is used to approximate the yield stress for a given geometry, and subsequently for inverse design of the system with predefined strength characteristics. The predictive model identifies designs of yield strength 10.91 GPa, compared to a baseline random search which gave a maximum strength of 9.67 GPa. We find that the high strength geometries have inclusions which are stacked vertically along the axis of applied stress. Those of low strength are found to organize similarly, but where the row of pores is rotated 45 degrees out from this axis. Visually, the geometries of these two extremes can respectively be perceived as elevators and escalators.

How does chemical erosion change the pore structure of a rock?

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Chemical erosion is a complex phenomenon that can significantly change the pore structure of rocks. Recent advancements of X-ray microtomography increased the interest of the scientific community to study these in-situ changes of pore space. We have analyzed two limestone samples of the same rock: partially dissolved and undissolved, both collected from a local quarry in Smerdyna (Poland) where intense karstification is observed. We have obtained X-ray scans of these samples and used image processing methods to quantify the changes to the pore geometry induced by a natural dissolution. In particular, we have compared the distribution of local thickness of the pore and grain component in both samples, connectivity of their pore spaces and shapes of individual pores. Such a comparison allowed us to quantify the extent of homogeneity of the natural karstification process. Interestingly, we found that the changes in the pore and grain distribution are not coherent: mean pore size increment is higher than mean grain size decrement. We associate this effect with a prevalent role of merging between the pores in a natural dissolution process.

Recent advancements of X-ray microtomography imaging (XCMT) increased the interest of researchers to study the change in pore geometry of carbonate rocks due to dissolution. On the example of the image analysis of samples of a Miocene limestone which have been collected from a quarry located near Smerdyna (Poland) - after discussing the preparation of images itself - we will introduce quantities to quantify the local and global changes in the geometry of the pore space and the rock matrix caused by natural dissolution. We will present the results of our measurements of porosity, thickness, anisotropy and connectivity obtained with the BoneJ software and discuss the resulting arguments for heterogeneity of the natural dissolution process.

GIAMAG magnets for magnetic nanoparticle manipulation in life sciences

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Abstract

In order to realize magnets with efficient magnetic separation capabilities, it is important to have a strong force $\boldsymbol{F_M}$ acting on the magnetic bodies. $\boldsymbol{F_M} \propto \boldsymbol{B}\nabla\boldsymbol{B}$, where $\boldsymbol{B}$ is the magnetic field strength and $\nabla\boldsymbol{B}$ the magnetic field gradient. Many permanent magnets on the market have large magnetic fields, but relatively weak field gradients.

A new design of a magnet system denoted GIAMAG (GIAnt MAgnet field Gradient) has been patented by one of the authors [1] and realized [2] with an unprecedented value of the field gradient $\nabla\boldsymbol{B}$. Several patents and applications protect the magnet technology [3]. Existing magnet systems can just pull efficiently magnetic microparticles from solutions, whereas GIAMAG can extract magnetic particles down to nanosizes. The principal design of GIAMAG is outlined in figure 1.

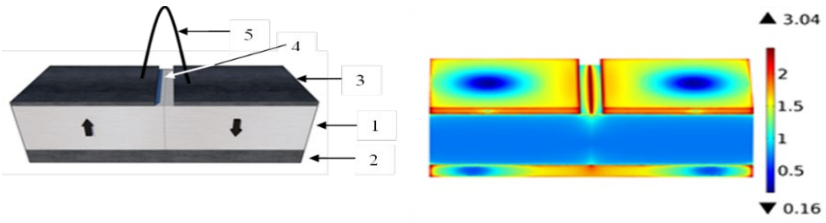

Figure 1. Left: Schematic outline of the original design of the GIAMAG magnet. The system consists of the following key components: Two adjacent permanent magnets (1) with opposite direction of magnetization, a yoke (2) and masks (3). The design involves a small gap (4) producing a very strong magnetic field gradient (5). Right: Computer simulation of the magnetic field strength distribution on the surface with N52 grade Neodymium–iron–boron magnets. The color scale is given in Tesla.

Simulations have been performed on the various geometries. Typically, one obtains values of $\boldsymbol{B} \cdot \nabla\boldsymbol{B} \sim 500 - 1000$ Tesla^2/m. This is roughly a factor of at least 10 up from conventional magnet separation set-ups.

GIAMAG offers unique possibilities in the following research and development areas:

- Separation of magnetic beads is a major technology used for diagnostic applications or drug monitoring
- Industry is moving from microparticle size to nanoparticles, to improve output and quality of diagnostics (precision medicine); Improved magnet designs and processes needed on nano level
- Use of nanoparticles open for new diagnostic tools, e.g., ctDNA isolation for cancer diagnostics. There is a need for automation and standardization to bring ctDNA to a routine diagnostic use

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Hybrid non-equilibrium patterns by coupling of dissipative electric driving and magnetic fields

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Non-equilibrium states lead to emergence of novel functionalities that are not achievable in thermodynamic equilibrium, such as self-assemblies and switchable dynamics. Despite their technological importance, designing materials with dissipative functionalities remain challenging since they are inherently complex. Therefore, developing non-equilibrium systems is fundamental. In our recently published work, we introduce a system consisting of electroferrofluid; an electrically and magnetically responsive dispersion of nanocolloids, and demonstrate that steady-state concentration gradients with diffused interfaces can be driven by electric fields in low electric field regimes [1]. We demonstrate the formation of patterns with well-defined periodicities by applying magnetic fields to the voltage-controlled concentration gradient [1].

In addition, in high electric field regimes, stationary undulating patterns, time-varying spatiotemporal states and chaotic behaviors are observed. Furthermore, a wide variety of tunable hybrid non-equilibrium states can be achieved by coupling of electric and magnetic fields, leading to various patterns and structures. Moreover, we demonstrate that minute changes in traces of water modifies the electric responsivity of the electroferrofluid, which can then affect the emerged patterns, which points towards the complexity of the system. This experimental study and the utilized concept of driving hybrid dissipative states by coupling of magnetic and electric fields, bring means and inspiration towards designing materials with adaptive functionalities.

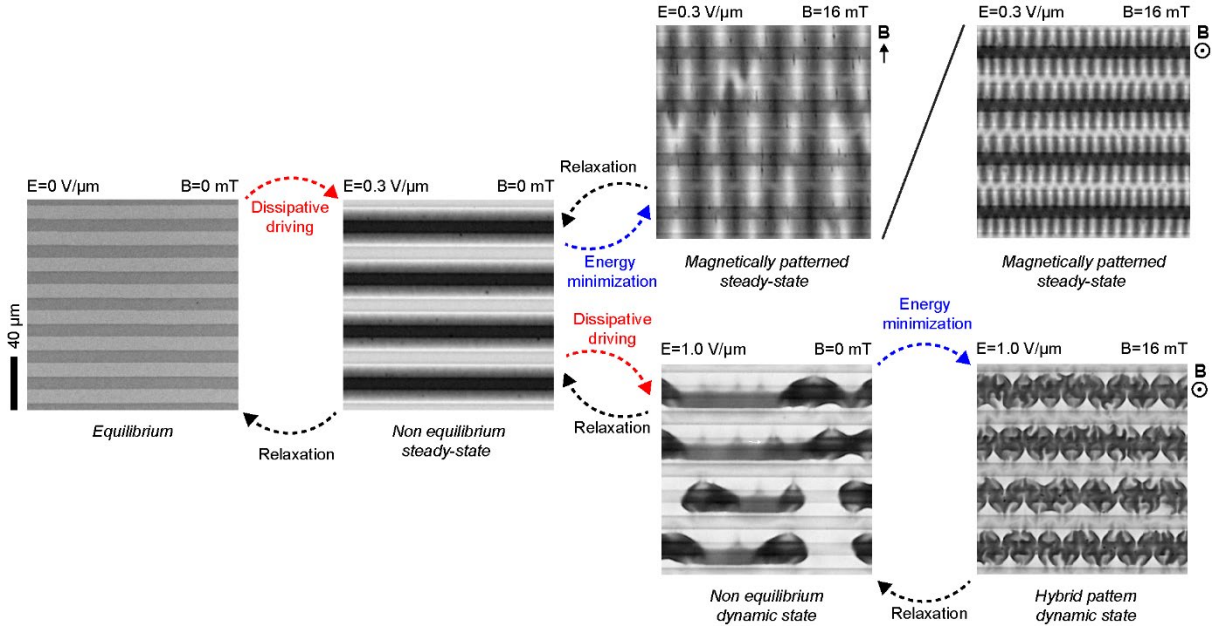

Figure 1: Examples of various emerged non-equilibrium states.

[1] T. Cherian, F. Sohrabi, C. Rigoni, and J. V. I. Timonen, *Sci. Adv.* **7**, 52 (2021).

Confinement-mediated collective motion of biased swimmers: magnetotactic bacteria in channels and droplets

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Magnetotactic bacteria (MTBs) align passively to external magnetic fields due to the presence of nanomagnets in their cytoplasm, and motile MTB strains are therefore biological instances of biased microswimmers. Experimentally, suspensions of MTB self-organise and create large-scale flows when confined in channels or droplets. We model these confined suspensions using hydrodynamic singularities and their images, and successfully reproduce the observed dynamics and flows. In a channel, plumes of swimmer form as they accumulate on a plane wall and generate convection-like flows. We find that these plumes stem from the clustering of hydrodynamic force dipole swimming against a wall. In a sphere on the other hand, the large-scale flow is a global vortex with a preferred direction orthogonal to the magnetic field. The interaction between force dipole and boundaries is again necessary for the vortex formation, but we show that the rotation direction is set by the interplay of gravity and swimmers' chirality.

Limit cycles turn odd metamaterials into robots

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Active systems are not constrained by the principle of energy conservation, allowing for a wide variety of wave phenomena not accessible to ordinary passive matter. By implementing local non-conservative interactions between particles within a network, complex collective behavior can result, providing new avenues in material design.
In particular, active elastic materials can be made by considering Hookean couplings which depend on the actuation direction, breaking chiral symmetry. A corollary of this non-reciprocity is that the work around a closed loop of deformations is generally nonzero.
To probe this departure from classical elasticity, I consider a simple building block made from robotic units equipped with sensors and actuators, exhibiting work cycles without external driving, i.e. due to self-oscillation. Chains of these robotic units demonstrate interesting functionalities such as locomotion and impact control when coupled to the environment by leveraging the uni-directional waves that propagate through it.
Furthermore, a 2D lattice with embedded active rings exhibits odd elastic properties as well as non-Hermitian skin waves showcasing a relationship between microscopic couplings and macroscopic properties. Altogether, these systems of distributed robots represent an ideal platform to study, engineer and control the emergent properties of active systems facilitating the development of autogenous smart materials, topological sensors and noise suppression schemes.

Antimicrobial nanoparticles: discovering kinetic pathways to improve stability through time-resolved synchrotron SAXS

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Abstract

Antimicrobial peptides (AMPs) are not yet readily suitable for systemic delivery in therapeutic applications, as they have low retainability, are degraded, and are cytotoxic. This research aims to find and define systems to effectively encapsulate the AMP colistin with the block copolymer poly(ethylene oxide)-poly(methacrylic acid) (PEO-b-PMAA), through complex coacervation, to reduce the side effects of colistin treatment. During complex coacervation, neutral complex coacervates are formed, which contain colistin. It is essential to understand the kinetic pathways for peptide-polymer coacervates to control the structure and stability and to determine the optimal procedure to prepare reproducible nanoparticles. We have obtained (preliminary) stopped-flow-time-resolved SAXS results which revealed that at stoichiometric charge ratio 1:1, the colistin and the polymer form very stable and reproducible complex coacervates with a defined structure during mixing, within milliseconds. Modeling shows that after mixing, the molecular weight and size of the complex coacervates increases gradually over time, until a plateau is reached at 2 seconds, seemingly following classical nucleation theory.

Liposome-assisted in-situ delivery of biomembrane-impermeable cargo to artificial cells

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Key words: cargo delivery, liposome, giant unilamellar vesicle, membrane fusion

Abstract

We report on liposome-mediated targeted delivery of membrane-impermeable constituents into surface-adhered giant lipid compartments, employed as model artificial cells. We perform the delivery by means of an open-space microfluidic device, which perfuses the individual lipid compartments with cargo-loaded small unilamellar vesicles (SUVs) composed of cationic lipids. We first monitored the fusion dynamics via Förster resonance energy transfer (FRET) upon labeling the membrane of the small vesicles, as well as the membrane of the targeted giant lipid compartments with FRET fluorophore pairs. We then showed that upon fusion, water-soluble dyes, fluorescently labeled genetic polymers, sugars and proteins carried by the SUVs, can be successfully internalized by the giant lipid compartments. Finally, by encapsulating carbonic anhydrase (CA) inside the giant lipid compartments, the enzymatic hydrolysis of carboxyfluorescein diacetate (CFDA) was achieved, resulting in the increased fluorescence intensity of the product carboxyfluorescein (CF). Subcompartmentalization phenomenon was observed during the liposomal delivery of the enzyme, leading to different amount of CF formation in each subcompartment. We intend to apply this delivery technique to artificial cells to perform chemical reactions and cell-free gene expression, and to gain a deeper understanding of possible chemical activity and communication within the primitive cell populations.

Determining elastic constants and non-equilibrium director configurations of nematic liquid crystals using artificial neural networks

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(Dated: March 2022)

Supervised machine learning and artificial neural network approaches can allow for the determination of selected parameters or the structure of a material from a measurable signal without knowing the exact mathematical relationship between them. Here, we demonstrate that from the time-dependent intensity of the transmitted light under crossed polarizers through the reconfiguring nematic liquid crystal (NLC), the nematic elastic constants and the initial configuration of the director can be found using neural networks. Specifically, the relaxation from a random (qeunched) initial state of the NLC to the minimum free energy state is numerically simulated multiple times, using Frank-Oseen free energy minimisation, for random values of elastic constants, and simultaneously, the transmittance of the NLC sample for monochromatic polarized light using the Jones matrix formalism. The obtained time-dependent light transmittances and the corresponding elastic constants form a training data set, on which the neural network is trained. This allows determining the elastic constants for different types of liquid crystal cells and nematic geometries. Finally, we demonstrate that the numerically trained neural network can also be used to determine elastic constants from full experimentally measured data.

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6 Geilo School 2022 group photo