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Gulliver

EXPERIMENTAL AND THEORETICAL TRAVELS IN SOFT MATTER

2025 - 2026

TOPICS

ACTIVE MATTER

ACTIVE MATTER AND COLLECTIVE EFFECTS

COLLECTIVE PHENOMENA

SOFT MATTER

STATISTICAL PHYSICS

THEORETICAL METHODS

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O. Dauchot

V. Démery

M. Fruchart

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Three is a crowd: Many-Body Correlations and Tuning Behaviour in Zebrafish

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Financement: candidature à l'EDPIF

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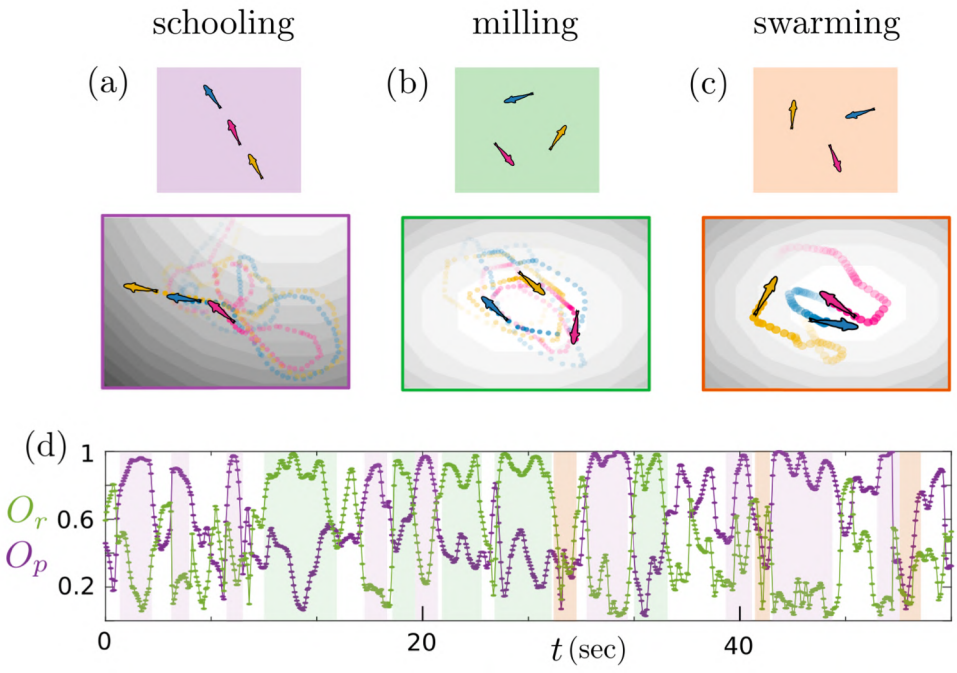

Figure. States in the zebrafish system. (a) Schooling, high polarization O_p, (b) milling, high O_r and (c) swarming low O_p and O_r. (d) Time-evolution showing multistate system behaviour.

Résumé

Collective behaviour in biological systems and its connections to phase transitions in physical systems has driven much of the current surge of interest in active matter. From birds to midges to bacteria, a variety of phenomena across a range of lengthscales have been investigated.

While collective behaviour in fish has received some attention, less is known where the fish are tracked in 3d. This project develops our existing work modelling experimental data with simple active matter models, to more sophisticated models which include perception [1,2].

The key aims of this project are as follows:

- We have recently shown there is no fundamental difference in behaviour in groups of 3-50 fish – “three is a crowd” [2]. But how does this change in larger groups? Are the normal order parameters even appropriate to larger groups?

- We have been able to tune the swimming in zebrafish through genetic modification [3]. The swimming behaviour is changed, but can the mutant fish be described within the same modelling framework as the wild type?

[1] Yang Y *et al, PLOS Comp. Biol*. 18 e1009394 (2022).

[2] Zampetaki A, et al *Nature Commun* **15** 2591 (2024).

[3] Yang Y *et al,* In press, *PLOS Comp. Biol*., BioRXiv doi.org/10.1101/2024.04.02.587671 (2024).

Keywords: active mater, active colloids, self-assembly, phases of matter

New Phenomena in Active Matter in 3D

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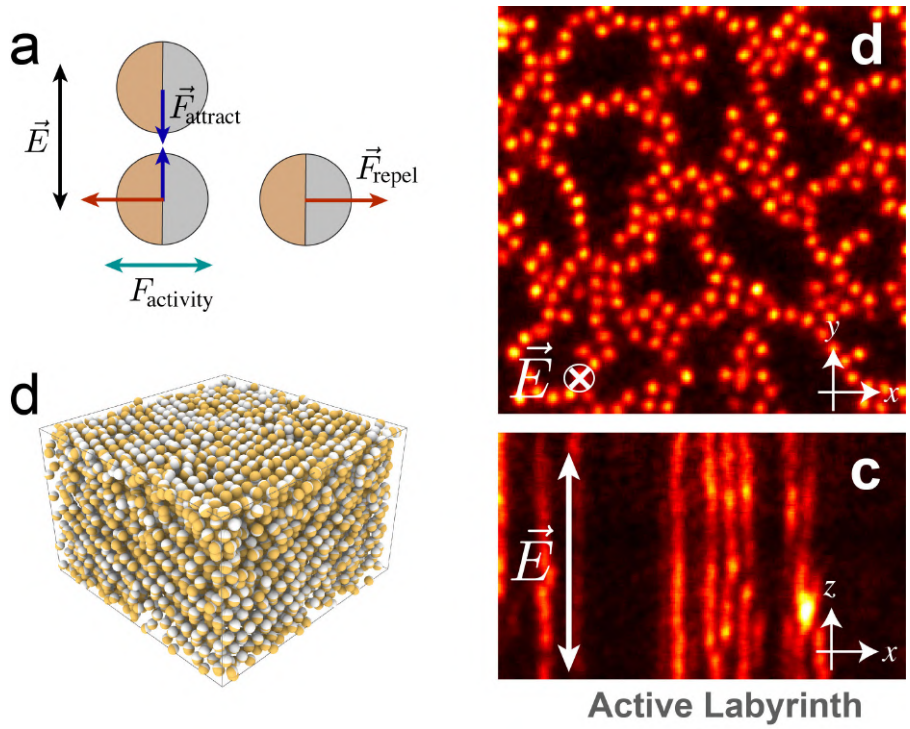

Figure. Active colloids in 3d. (a) The electric field E provides the activity in the *xy* plane. It also induces dipolar interactions, an attraction in *z* and repulsion in *xy*. (b,c) Snapshots of new phases of matter using 3d confocal microscopy. (b) *xy* plane showing labyrinth (active membrane). (c) xz planes. (d) Active colloidal crystal, experimental data rendered showing Janus particles organised into phonon-like waves.

Résumé

Active matter is one of the most exciting fields in condensed matter physics. Much of the excitement comes from the discovery of new phenomena, and the connection to biological systems. While modelling biological systems – such as fish – enables insight into new domains of physics [1], quantitative understanding from first principles is challenging to put it mildly. **Imagine a physical system with behaviour similar to biological systems and yet whose properties can be predicted in a well-controlled manner**: such a system is active colloids [2]. These micron-sized particles exhibit a unique combination of thermal motion (so they follow statistical mechanics) and activity (so they exhibit new phenomena).

We have discovered a variety of new and unexpected phenomena in the active colloids, from hydrodynamic coupling akin to excited states in molecules, novel active polymerisation [2]. We have recently developed the first 3d active colloidal system (see figure) which we can study both in experiment [3] and with computer simulation [2]. This project aims to explore this system, from the role of activity in crystal nucleation and self-assembly to investigation of new phenomena such as phonon-like waves.

[1] Zampetaki A, Yang, Y, Loewen, H and Royall CP " Dynamical Order and Many-Body Correlations in Zebrafish show that Three is a Crowd" *Nature Commun* **15** 2591 (2024).

[2] Chao X, Skipper K, Royall CP, Henkes S, Liverpool TB, "Traveling strings of active dipolar colloids", Phys. Rev. Lett. 134 018302 (2025).

[3] Sakaï N, Skipper K, Moore FJ, Russo J and Royall CP, "Active Dipolar Colloids in Three Dimensions: Non–Equilibrium Structure and Re-entrant Dynamics", Soft Matter, 21, 5204 (2025).

Keywords: active matter, active colloids, self-assembly, phases of matter

Mechanical Response of Active Solids

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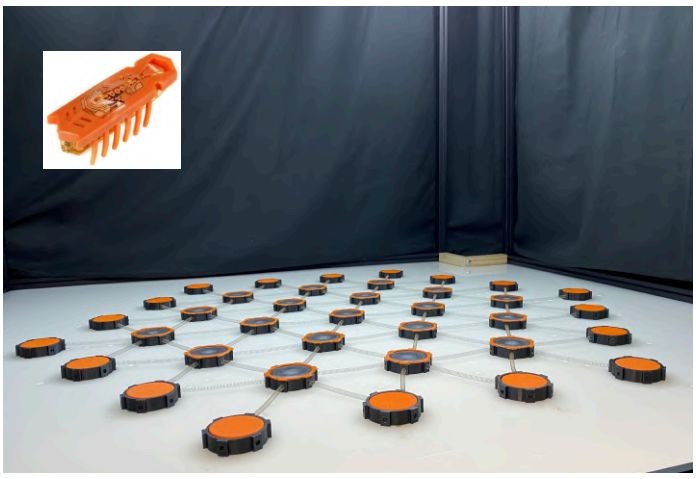

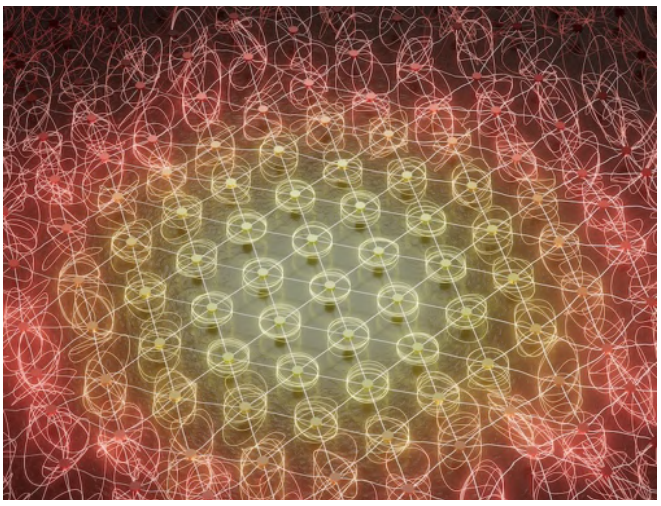

Figure. Active elastic lattices and Collective Actuation

ACTIVE MATTER AND COLLECTIVE EFFECTS

Résumé

Active matter describes systems in which the elementary constituents consume energy to produce work. In active liquids, this work is turned into motion and the interactions lead to fascinating collective motion, as widely observed in nature, from bird flocks to cellular cytoskeletons.

In active solids, the elementary constituent are embedded in an elastic matrix in which they exert local stresses. These stresses deform the matrix. The induced strain in turn acts on the active units. As a result of this retro-action one observes spontaneously oscillating solids. Eventually, designing the elastic matrix and its coupling to the active units, one could program a new type of functional materials.

In the past three years we have tailored an artificial system that combines activity and elastic architecture and demonstrated that selective and collective actuation is a hallmark of active solids https://twitter.com/i/status/1561626005520932864. These results open a brand-new avenue of research, from further experimental and numerical investigations to theoretical analysis.

During this internship we would like to study **the mechanical response of such solids.** Preliminary observations reveal **extremely anomalous elasticity**, with mechanical response in the direction orthogonal to the stimulus!

Depending on the personal taste of the intern, and the progress of the project, the internship can be mostly experimental, or numeric, or theoretical. In all cases, we will take advantage of our existing set-up as well as the good numerical models of these systems.

Keywords: active matter, elastic lattices, mechanics, etc…

Colloid Nucleation: the « second-biggest discrepancy in physics »

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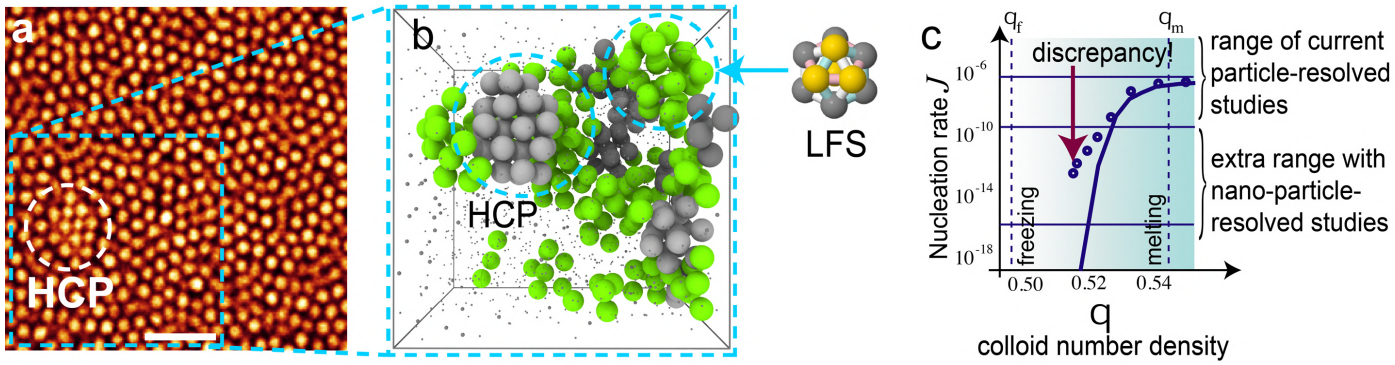

Figure. (a) Crystal nucleating in a liquid of colloids. 3d Confocal microscopy image. Bar=20μm. (b) 3d rendering of particle coordinates: grey hexagonal close-packed crystal, green liquid locally favoured structure. (c) Nucleation rate in hard spheres. Line – prediction from computer simulation, data points, experimental data.

Résumé

How does a liquid transform into a crystal? Remarkably, even now this everyday process is poorly understood. One challenge with studying the birth of a crystal, the process of nucleation, is that it is hard to see such tiny groups of a few atoms or molecules. Mesoscopic colloidal particles follow the same laws of statistical mechanics and form crystals just like atoms. Early work with colloids found, very surprisingly, that the rate of formation of crystal nuclei J is low, can be *ten orders of magnitude* faster than the prediction from computer simulation, “the second-biggest discrepancy in physics” (Fig. c) [1].

Now it is possible to see the colloidal particles in a confocal microscope, which can image in 3d (Fig. a). This is a very useful method to investigate nucleation, because we can directly see the nucleus and track the coordinates of the particles (Fig. 1b) [2]. This data can be directly compared with the results from advanced rare event computer simulations [3]. This project can be either experimental or computational.

[1] Royall CP, Charbonneau P, Dijkstra M, Russo J, Smallenburg F, Speck T and Valeriani C. “Colloidal Hard Spheres: Triumphs, Challenges and Mysteries”, Rev. Mod. Phys. 96 045003 (2024).

[2] Kürten L, Castagnède A, Smallenburg F, Royall CP, "The Free-Energy Barrier of Precritical Nuclei in Hard Spheres is Consistent with Predictions"

[3] Taffs J and Royall CP “The role of fivefold symmetry in suppressing crystallisation”, Nature Communications 7 13225 (2016).

Keywords: colloids, nucleation, confocal microscopy

Swimming droplets in chemical gradients

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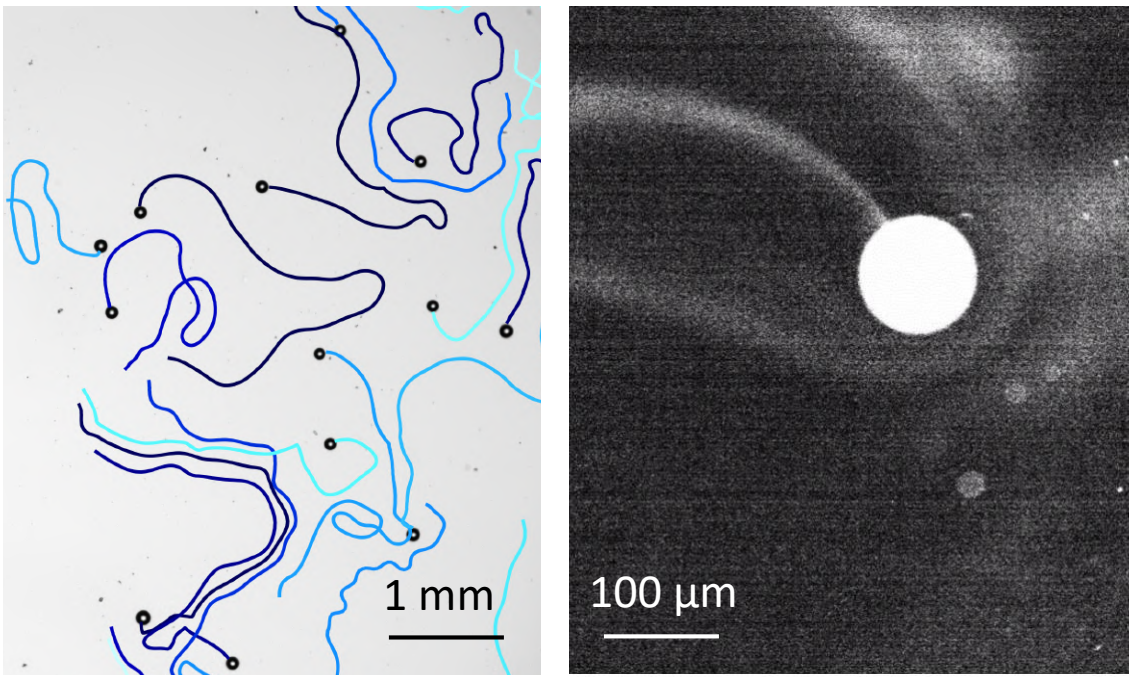

Figure. Trajectories of swimming droplets showing complex behaviors (left). Fluorescein initially present in the droplets in the droplet allows to follow the path of a droplet (right). Droplets are really sensitive to their environment.

Résumé

Artificial micro-swimmers have recently become a central field of research in soft-matter, the reason being that they open the way towards numerous applications at small scales, including fluid pumping, sensing and capture of molecular species, transport and cargo delivery.

A very promising and original type of swimmer developed in our team, consists in pure water droplet swimming in an oil phase containing micelles of surfactant. The swimming mechanism and motion of these droplets have been investigated in details in the past few years [1]. We have studied the swimming behavior of such micro-droplets in confined conditions in capillary tubes. We have observed non-conventional spontaneous fragmentations under extreme confinement that we have related to the interfacial activity of the system [2]. More recently, we have investigated the behavior of such droplets facing a counterflow or swimming against gravity. The swimming velocity of such droplets is dependent on their nearby environment.

We propose to investigate the behavior of such droplets facing well-controlled chemical barriers using microfluidics. We will use the facilities offered by the Institute Pierre Gilles de Gennes to create well controlled microchannels. The experiments will be then carried in the Gulliver lab.

We are looking for a highly motivated student, with a good background in soft matter physics. Important concepts to be at ease with are surface tension and hydrodynamics. Experimental skill in microfluidics and ease with image analysis is an advantage, but is not mandatory.

[1] Z. Izri et al., PRL 113, 248302 (2014).

[2] C. de Blois et al., Soft Matter,17, 6646 (2021).

Keywords: soft matter, hydrodynamics, microfluidics, microdroplets, microfabrication.

Advection and diffusion in complex, near-surface media

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Financement: Oui

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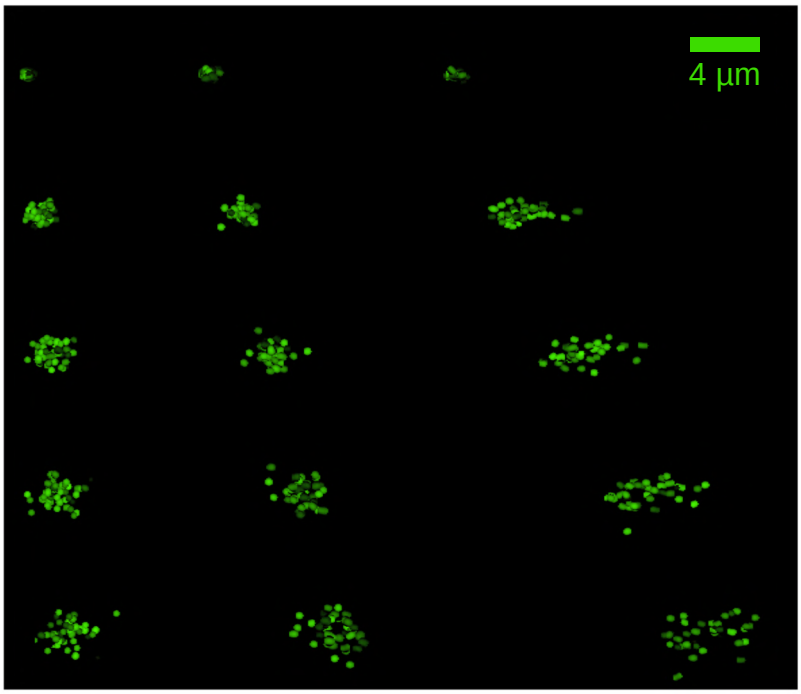

Figure. Near-surface nanoparticle dynamics observed using total internal reflection fluorescence. The columns are time series (Δt = 12 ms) for larger and larger mean velocities in a microfluidic flow. Detailed analysis of the dynamics of these particle clouds provide diffusive and advective dynamics.

Résumé

The dynamics of disordered systems are ubiquitous in condensed matter physics, from glasses to intracellular media. The former example is one of a complex, multicomponent mixture [1] undergoing constant decomposition and regeneration thanks to biochemical and physicochemical energy inputs. Within this mixture, each species is transported according to its local environment, comprising local fluctuations and global movements imposed by external stresses – due to an external flow, say. Taking as an emblematic object within this transport scenario, a protein molecule is an object with scale 10^1 nm, always near surface and subject to advective and diffusive motions.

During this internship, we will experimentally study an abstract and controlled version of the the complex intracellular scenario described above. Fluorescent nanoparticles take the role of a biomacromolecule, microfluidic channels are used to provide interfaces and global flow [2], while dual input channels serve to prepare non-equilibrium mixtures akin to the intracellular matrix. Referring to the Figure at left, we use particle tracking to observe (i) the microscopic and local diffusive dynamics [3], and (ii) the advective transport there. To observe these phenomena, we use the experimental and surface-sensitive technique total internal reflection fluorescence microscopy. We thus achieve 3D, nanometrically resolved particle dynamics in near-wall, microfludic flows. Our study will bring first measurements on the impact of realistic phase decomposition dyamics at the particle level in these emblematic complex flow scenarios.

[1] J.D. McGraw, Europhysics News, **56**, 13 (2025)

[2] G. Guyard et al , Soft Matter, **17**, 3765 (2021)

[3] A. Vilquin et al., PRL, **130**, 038201 (2023)

Keywords: soft matter, hydrodynamics, statistical physics, complex fluids, diffusion

Models and algorithms for the next generation of studies of molecular glass transitions

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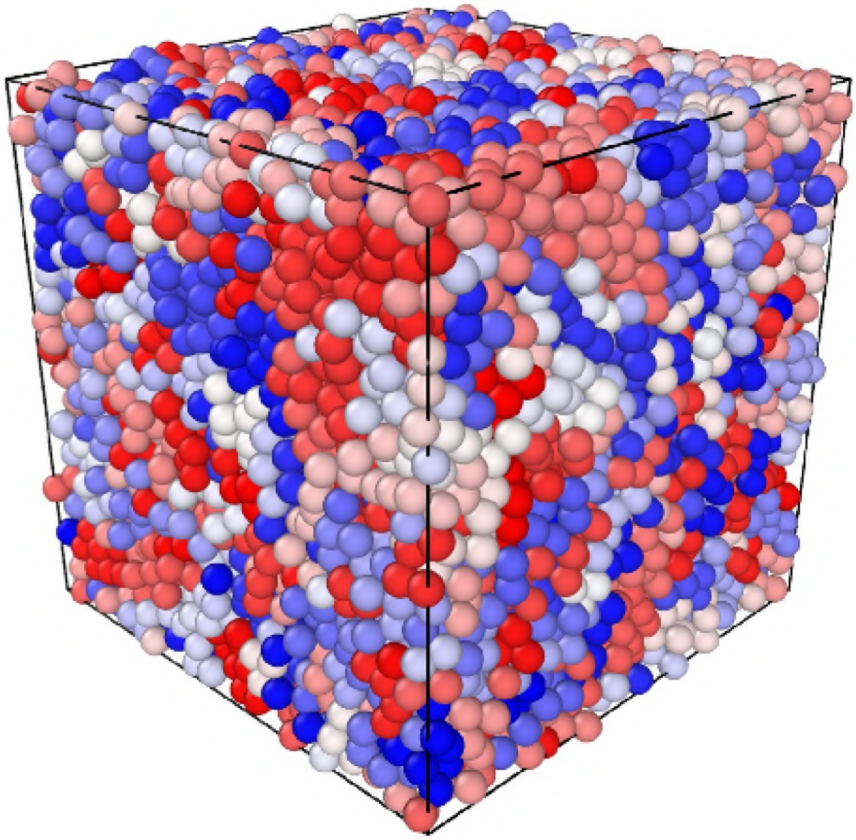

Construction of a computer model for polymer glasses for which enhanced sampling of configuration space can be performed using non-local Monte Carlo techniques.

Résumé

Most liquids gradually solidify at low temperature via a physical process called the **glass transition** towards a non-equilibrium disordered state of matter. This process is well-known experimentally, and is routinely observed in a variety of molecular and macromolecular fluids. The practical relevance of glassy materials in everyday life is obvious. Despite decades of research it remains very difficult to accurately predict the physical properties of these systems. To this end, it would be desirable to use computer simulations to address these questions, but **state-of-the-art models and computational techniques are limited**. A large gap remains between experimental work on real systems and conventional simulations. Our goal here is to fill this gap.

Recently, we developed a family of new models for atomistic glasses (relevant for metallic and colloidal glasses) together with Monte Carlo techniques that can provide an enormous computation speedup, reaching 10 orders of magnitude in some cases. In this thesis, we will develop, in the same spirit, a family of new models for molecular fluids together with efficient Monte Carlo techniques to easily sample their complex configuration space, and accurately predict physical properties.

As a first step, we will construct models for **a variety of molecular architectures**, from simple shapes (dumbbells, pyramids, tetrahedra etc.) to macromolecular chains (oligomers, polymers). In parallel, we will invent and optimize **non-local Monte Carlo techniques** to efficiently reach thermal equilibrium and sample configuration space. Armed with these new models and techniques, a series of **fundamental physics questions** will be addressed using computer simulations, regarding the relaxation dynamics and the structural and mechanical properties of molecular fluids. **Comparison with experimental work** will also be performed.

Keywords: statistical mechanics, glassy dynamics, computer simulations

Is there a phase transition between a liquid and a disordered glass?

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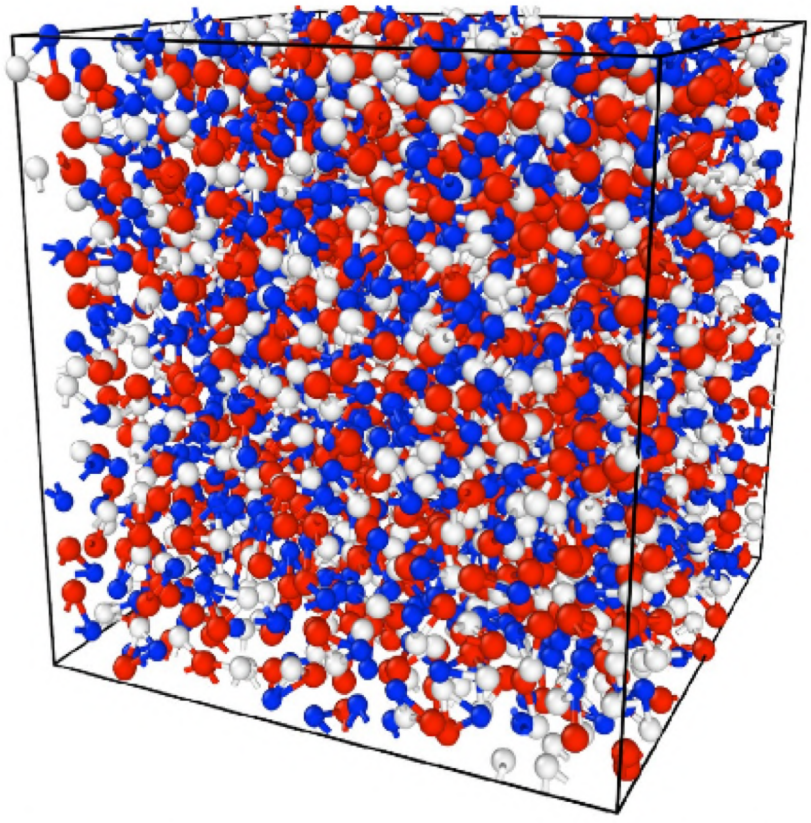

This molecular fluid transforms at low temperatures into a non-equilibrium glass state. Is this process controlled by an underlying equilibrium phase transition described by statistical physics?

Résumé

Most liquids gradually solidify at low temperature via a physical process called the **glass transition** towards a non-equilibrium disordered state of matter. This process is well-known experimentally. At the fundamental level, however, its **statistical mechanics** description is much less advanced, as it took several decades of difficult analytic work to recently derive a solid mean-field transition of the liquid-glass transition, now reaching completion. The effect of fluctuations in disordered systems is typically very important, but theory remains unable to attack this problem. In the last 10 years, considerable progress was also made to develop simple yet realistic models for glass transition studies, as well as numerical methods to more **efficiently sample the complex configuration space** of glassy models.

State-of-the-art theory and simulations suggest that an equilibrium phase transition between liquid and glass states could exist in model liquids in finite dimensions, but demonstrating the existence of the transition and studying the associated properties (universality, exponents, characteristic lengthscales) has not been possible so far, leading some researchers to claim that this is an impossibly difficult task. We wish to solve this difficult problem.

In this thesis, we will develop and combine numerical approaches to systematically investigate the nature of the transition between liquid and glass states in equilibrium conditions. By carefully choosing simple glass models, and starting with modest system sizes, we will develop **computational approaches to very efficiently explore complex energy landscapes and cross the equilibrium liquid-glass Kauzmann transition for bulk systems**. In a second step, we will investigate whether findings in small systems extend to larger ones, in order to develop finite size scaling methods to approach the thermodynamic limit. Ultimately, this work will provide a definitive answer to a mystery that has haunted the field of disordered systems for more than fifty years by demonstrating whether a glass state of matter can truly be defined in three-dimensional glass-forming liquids.

Keywords: statistical mechanics, glassy dynamics, computer simulations

Physics models for the origins of Darwinian evolution

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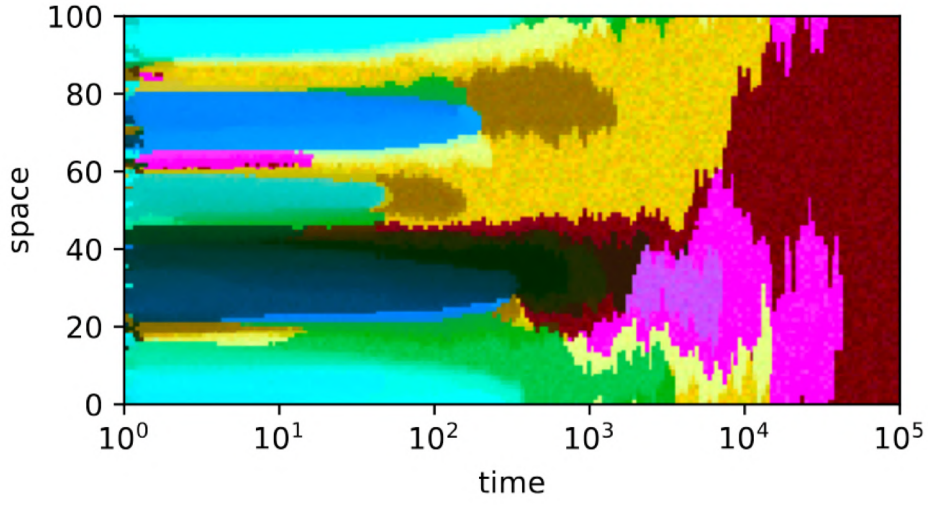

Spatio-temporal dynamics of one of our models. This model is defined in a one-dimensional space (y-axis). At each point in time and space, different molecules are present. The colors represent different combinations of molecules, with similar colors representing similar combinations. As time passes (x-axis, on a log scale), some compositional states appear, disappear, or expand at the expense of others in a process analogous to Darwinian evolution.

Abstract

Life is understood to be both the result and the engine of Darwinian evolution. Darwinian evolution occurs when three ingredients are present: (1) Variation: a population of individuals exhibits different traits. (2) Inheritance: these individuals reproduce and pass on their traits, at least in part, to their offspring. (3) Differential reproduction: some traits lead to greater survival and reproductive success than others.

In modern life forms, the mechanisms underlying these properties are complex and themselves the products of Darwinian evolution. At the origin of life, however, Darwinian evolution must have emerged from simpler processes. What could they be? We approach this question from a physics perspective, aiming to identify physical processes that can possibly give rise to Darwinian-like evolutionary dynamics beyond the specific pathway that led to life on Earth [1].

To this end, we develop and analyze statistical physics models. We recently proposed a novel class of models [2] in which systems of coupled chemical reactions exhibit key features of Darwinian evolution, such as diversity, selection, inheritance, and adaptation, despite the absence of autocatalysis, assembly processes, or compartments, which are often considered essential. Our goal is to further develop these models to understand how other key biological features, such as complex information processing, hierarchical organizations and individuality, can emerge.

[1] N. Goldenfeld & C. Woese (2011). *Life is physics: evolution as a collective phenomenon far from equilibrium.* Annu. Rev. Condens. Matter Phys., 2 : 375-399.

[2] G. Bunin & O. Rivoire (2025). *Evolutionary features in a minimal physical system: diversity, selection, inheritance, and adaptation.* PNAS 122 : e2425753122.

Keywords: origin of life, nonequilibrium dynamics, stochastic processes

Toy models of protocells for the origin of life

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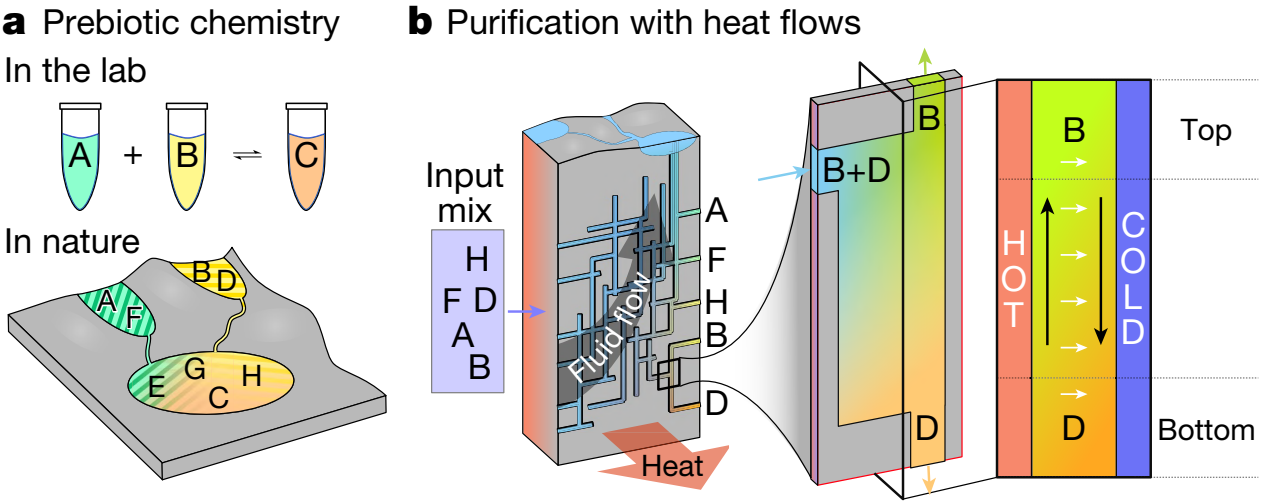

(a) Prebiotic chemistry reaction requires precisely timed mixing and reaction of well-defined products. In nature, starting solutions are complex mixtures that produce many undesirable products. (b) Ubiquitous heat flows form a geo-microfluidic system that can separate chemicals in the presence of fluid convection (black arrow). Figure taken from Ref [1].

Summary

We plan to build a thermodynamically consistent model of a protocell, to understand some aspects in the Origin of life (OL). We will incorporate metabolic reactions in a highly coarse-grained way which we will couple to an energy flux, produced by a (thermal of chemical) gradient between the outside and inside of the protocell.

During this internship, we would like to characterize the heat or dissipation current that exist together with matter currents and explore theoretically how this heat current can drive the selection for certain products in this non-equilibrium system. We expect that the strength of the selection should be related to the thermodynamic efficiency that bounds the heat current.

On the numerical side, the model will be numerically solved using a recently developed finite elements software package. The results will be compared to experiments carried out in the group of D. Braun at University LMU in Munchen [1].

This project builds on previous works carried out in the group on the topic of the Origin of Life: on the the emergence of homochirality in large chemical reaction networks [2], on the identification of autocatalysis within large chemical networks [3] and on transient compartmentalization dynamics [4]. This theoretical internship will benefit from strong interactions with experimentalists in ESPCI and with M. Castellana at Curie Institute.

[1] Heat flows enrich prebiotic building blocks and enhance their reactivity, T. Matreux et al., Nature, vol 628, 110 (2024).

[2] Emergence of homochirality in large molecular systems, G. Laurent, D. Lacoste, and P. Gaspard, Proc. Natl. Acad. Sci. U.S.A., 118, (2021)

[3] Universal motifs and the diversity of autocatalytic systems, A. Blokhuis, D. D. Lacoste, and P. Nghe, PNAS, 117, 25230 (2020).

[4] Selection dynamics in transient compartmentalization, A. Blokhuis, D. Lacoste, P. Nghe and L. Peliti, Phys. Rev. Lett., 120,158101 (2018)

Keywords: origin of life, thermodynamics, statistical physics

Statistical simplicity of random chemical reaction networks

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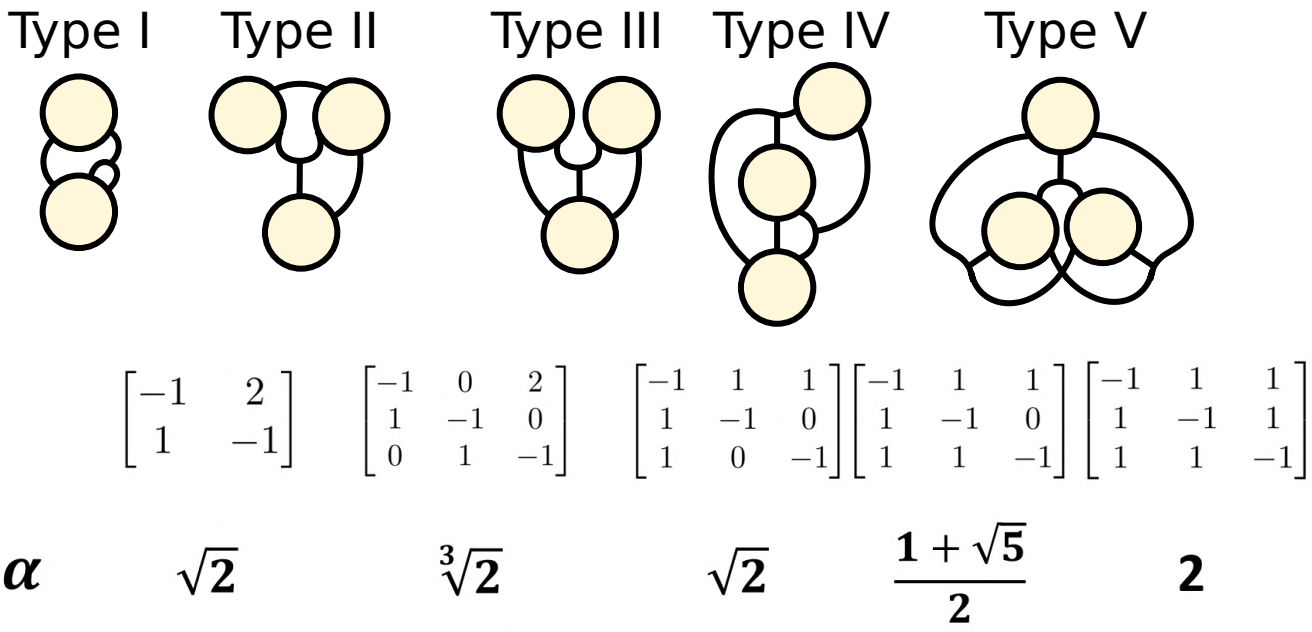

Five minimal autocatalytic motifs (figure taken from [2]). Yellow circles represent species, black lines connecting them represent reactions. Below, their associated stoichiometric matrices are shown together with their stoichiometric growth factor (bottom line).

Summary

Many systems in nature can be described using discrete input-output maps. A priori, there is no reason to expect that randomly chosen inputs are more likely to generate one output instead of another one. In ref. [1] however, using methods of algorithmic information theory, it was shown that the probability to obtain a given output from randomly sampled inputs is biased towards output of low complexity in the sense of Kolmogorov. This simplicity bias was found in various systems ranging from the folding of RNA to financial data and to the parameter-function maps in neural networks.

In this internship, we aim to extend these ideas to random chemical networks and investigate whether a similar bias towards networks of low complexity and high symmetry exists there.

We are particularly interested in a specific class of chemical networks, namely autocatalytic chemical reaction networks, because for these networks, we have previously identified specific minimal and topological motifs (see figure and Ref. [2]). These motifs appear frequently among random chemical networks of this type, suggesting a possible bias towards simplicity. Another question which we would like to investigate concerns the relation between the simplicity bias, the network robustness and thermodynamic constraints following our study in Ref [3]. Note that beyond chemical reaction networks, these methods may be also relevant to understand growth in economic systems [4].

The internship will take place in a mixed environment of theoreticians and experimentalists interested in various applications of Statistical physics to molecular programs, soft matter and living systems.

[1] Input-output maps are strongly biased towards simple outputs. K. Dingle, C. Q. Camargo, and A. Louis, Nature Com., 9, 71, (2018)

[2] Universal motifs and the diversity of autocatalytic systems, A. Blokhuis, D. D. Lacoste, and P. Nghe, PNAS, 117, 25230 (2020).

[3] Structural constraints limit the regime of optimal flux in autocatalytic reaction networks, A. Despons et al., Commun. Phys. (2024)

[4] Universal properties of autocatalysis, D. Lacoste and B. Ledoux, , chapter in book: 'Economic principles in cell biology' (2025), https://zenodo.org/records/15397884

Keywords: algorithmic information theory, chemical networks, statistical physics

Machine-Learning Force Fields and Simulation Methods for the Dielectric Properties of Water

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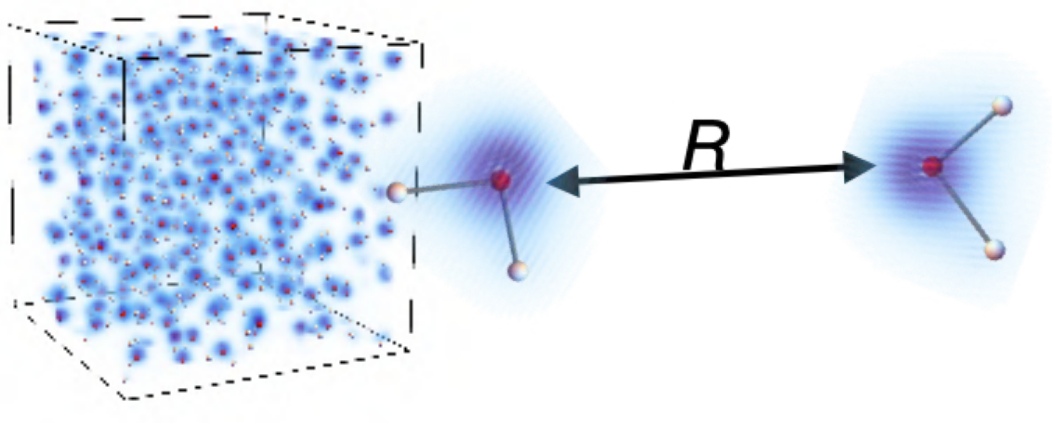
Possibilité de thèse: Oui

Financement: candidature à l'EDPIF



A) Water box simulated with AIMD-DFT. B) Characterization of the dielectric properties of neural network force field for water: long range and full electronic density.

Résumé

The dielectric behavior of water governs key processes in electrochemistry, nanofluidics, and materials science. While *ab initio* molecular dynamics (AIMD) captures its electronic structure accurately, it remains computationally demanding. Recently, **machine-learning force fields (ML-FFs)** trained on AIMD data have emerged as powerful tools to reproduce quantum accuracy at a fraction of the cost. However, their ability to describe long-range polarization and dielectric properties remains to be fully assessed and improved.

This internship aims to test and refine ML-FFs for liquid water. The student will perform molecular dynamics simulations using existing machine-learning potentials and compute dielectric observables including polarization correlations, charge structure factors, and frequency-dependent permittivity. These results will be compared with reference *ab initio* and classical simulations in order to assess the strengths and limitations of current ML approaches.

This internship is part of a broader project investigating the properties of the water/metal interface, including the capacitance and friction of water flowing over metal.

References A. Robert, H. Berthoumieux, ML. Bocquet, Phys. Rev. Lett. 130, 076201 (2023). J. Hedley, K.Bhatt, H. Berthoumieux, A. Kornyshev,, J. Chem. Phys. 162, 114703 (2025), D. Labavic, F. Brunig, R Netz, ML. Bocquet, H. Berthoumieux, arXiv2505.11101 (2025).

Keywords: Machine learning force field, water at the nanoscale

Polarization Functional for Water at the Electronic Scale

Encadrants:
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ML Bocquet (LPENS, ENS)

Possibilité de thèse: Oui

Financement: candidature à l'EDPIF

A.

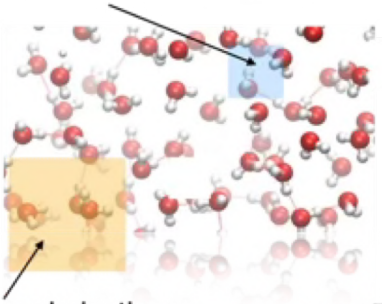
$$U_{el}[P] = U_{\text{Coulomb}}[P] + U_{\text{conf}}[P]$$

Coulomb interaction

Configuration energy

Functional of polarization P, analytic
calibrated on AIMD-DFT response function

B. P_1 intermolecular polarization mode (H-bond)



P_{el} P_{el} electronic polarization

P_2 polarisation for molecular clusters

$U_{\text{conf}}[\ P_1, P_2, P_{el}\ ]$

A) Electrostatic energy of water as a functional of the polarization.
B) Three polarization modes at different scales for water.

Résumé

Understanding the microscopic dielectric properties of water near metal surfaces is key to electrochemistry, catalysis, and nanofluidics. Recent experiments in nanoslits reveal interfacial water structure at subnanometer scales, calling for new theoretical models.
Water-metal interfaces are typically investigated using classical or ab initio molecular dynamics (MD) simulations. Breaking away from these purely numerical approaches, we have developed analytic functionals of the polarization to describe the dielectric properties of water at the nanoscale. These functionals are versatile, analytically tractable, and parametrized to reproduce dielectric properties of bulk water.
The goal of this internship is **to develop and parametrize a Landau–Ginzburg-type functional including electronic correlations.** By introducing coupling with confining metallic surfaces, we use these tools to describe the dielectric properties of confined water and to rationalize its unexpected experimental behavior.

References A. Robert, H. Berthoumieux, ML. Bocquet, Phys. Rev. Lett. 130, 076201 (2023). J. Hedley, K.Bhatt, H. Berthoumieux, A. Kornyshev,, J. Chem. Phys. 162, 114703 (2025), D. Labavic, F. Brunig, R Netz, ML. Bocquet, H. Berthoumieux, arXiv2505.11101 (2025).

Keywords: field theory, nanofluidics, confinement.