

New frontiers in liquid matter

Workshop in honor of the 80th birthday of

Jean – Pierre Hansen



July 4th to July 7th, 2022

Paris, France

Lydéric Bocquet

CNRS and ENS, France

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Acknowledgements :

The organizers are particularly grateful to Valérie Belle (CEA and CECAM-FR-MOSER), Dounia Benzouak (ENS-PSL), and Ingrid Unger (TU Wien) for their invaluable help in organizing this meeting and to Almaz Murshudova (TU Wien) for the layout of the booklet.

1. Description

Liquid matter physics has seen during the past decades a tremendous broadening, covering meanwhile not only physics, but also chemistry and biology, as well as -- from the methodological aspect -- mathematics and computer science. Concomitantly, the research activities which, admittedly, were originally rather motivated by academic curiosity have become relevant for numerous technological and practical applications, thanks in particular to the experimental developments now offering the possibility to fabricate and investigate complex soft matter systems at the single-particle level or to manipulate flows down to the nanoscale.

The idea of this workshop originated from the anticipation of Jean-Pierre Hansen's 80th birthday in May 2022. Jean-Pierre, now an emeritus professor in Paris, has played a key role in the development of liquid state theories and the simulation of liquid matter, as well as in establishing the CECAM community. From his early days in the group of Loup Verlet in Orsay (at the time where CECAM was created) to his European career in Paris, Lyon (he was among the founding fathers of ENS Lyon, where CECAM moved from Orsay) and Cambridge, he trained a large number of leading members of this community, at the interface between Physics and Chemistry, either directly or indirectly via his seminal books with Ian McDonald and Jean-Louis Barrat that influenced generations of new scientists in the field. His leading role has been recognized by many distinctions, including the Liquid Matter Prize of the European Physical Society in 2005 and the Berni J. Alder CECAM Prize in 2013.

The objective of this workshop is twofold. The first and obvious one is to celebrate Jean-Pierre's 80th birthday by gathering scientists who have interacted with him throughout his career. The second is to organize a high-profile scientific workshop focused on the latest developments of liquid matter related topics to which Jean-Pierre has made important contributions. This second objective will in particular be achieved by also inviting and accepting contributed talks from speakers without direct link with him but who illustrate the vitality of these fields, including: fundamentals of classical and quantum liquids, soft matter, charged systems and glassy systems.

Invited speakers:

- Rosalind Allen
- Ludovic Berthier
- Giulio Biroli
- Elisabeth Charlaix
- Marjolein Dijkstra
- Joachim Dzubiella
- Bob Evans
- Ramin Golestanian
- Angelos Michaelides
- Roland Netz
- Susan Perkin
- Stefano Sacanna

as well as special guests ...

Important dates:

- abstract submission: March 15th, 2022
- notification of acceptance: April 1st, 2022

Please note that due to technical reasons, before your participation in the event is accepted you can only apply for a poster, but all abstracts will be considered as possible contributed talks (20 minutes).

Practical information:

The conference will take place in Sorbonne Université (« campus Pierre et Marie Curie », formerly known as Jussieu — the metro station kept the same name). More details will be sent to registered participants in due time.

In order to prepare your contribution, please note that:

- plenary talks extend over 40 minutes (including discussion)
- contributed talks extend over 20 minutes (including discussion)
- posters walls will be available for presenting the posters (A0, vertical); posters will be on display during the entire workshop

2. Program

Day 1 – Monday, July 4th 2022, Opening session

12:30 to 14:00	Registration
14:00 to 14:10	Welcome & Introduction from the Organizers
14:10 to 14:30	Ignacio Pagonabarraga
	Welcome address - CECAM Headquarters
14:30 to 14:50	Thierry Dauxois
	Welcome address - CNRS and ENS Lyon

Session: Fundamentals of classical and quantum liquids

Chair: Jean-Louis Barrat

14:50 to 15:30	Robert Evans
	Density depletion and enhanced fluctuations in 'water' near hydrophobic solutes: identifying the underlying physics
15:30 to 15:50	Sophie Hermann
	Noether's theorem in statistical mechanics
15:50 to 16:10	Coffee break

Chair: Sara Bonella

16:10 to 16:30	Alberto Parola
	Thermal forces: from nanotubes to thermophoresis
16:30 to 16:50	Guillaume Stirnemann
	Toward a molecular picture of thermodiffusion of dilute aqueous solutions
16:50 to 17:10	Frédéric Caupin
	Reactive mixture as a model for fluids with water-like anomalies
17:10 to 17:30	Cecilia Herrero
	Connection between water's dynamical and structural properties: insights from ab initio simulations.
17:30 to 18:10	Angelos Michaelides
	Structure and dynamics of interfacial water

Day 2 – Tuesday, July 5th 2022

Session: Soft matter (Part I)

Chair: Mark Miller

09:00 to 09:40	Rosalind Allen Phase transitions in the growth of bacterial biofilms
09:40 to 10:00	Emanuela Bianchi Modeling and simulating charged patchy colloids
10:00 to 10:20	Ard Louis Why the world is simple: the algorithmic evolution of self-assembly
10:20 to 10:40	Coffee break

Chair: Giovanni Ciccotti

10:40 to 11:00	Hartmut Löwen Colloidal active matter
11:00 to 11:20	Natalie Malikova Organisation of charged nano-platelets and their aggregates in liquids and gels
11:20 to 11:40	Michiel Sprik Cahn-Hilliard theory for capacitive diffusion in colloidal fluids
11:40 to 12:20	Marjolein Dijkstra From theory of simple liquids to machine learning
12:20	Group Photo

Session: Glassy systems

Chair: Giorgio. Pastore

14:00 to 14:40	Ludovic Berthier Computer simulations of glassy liquids: what are the new frontiers?
14:40 to 15:00	Klaudia Milc Imaging and quantifying strongly confined flow of fat crystal dispersions with rheo-MRI
15:00 to 15:20	Laura Filion Unraveling structural and dynamical features in glassy fluids using machine learning
15:20 to 15:40	Coffee break

Chair: Michele Parrinello

15:40 to 16:00	Jean-Marc Bomont
	Overlap and glass quantization of the Gaussian core model
16:00 to 16:40	Giulio Biroli
	How amorphous materials yield under stress: a new kind of out of equilibrium phase transition

Chair: Paul Madden

16:40 to 16:50	Roland Netz
	The European Physical Journals – From scientists for scientists
16:50 to 17:10	Sauro Succi
	Life in the abyss: the hydro-structural connection
17:10 to 17:30	Jean-Pierre Hansen
	Some personal remarks
17:30 to 19:00	Poster session

Day 3 – Wednesday, July 6th 2022

Session: Confined systems**Chair: Marie Jardat**

09:00 to 09:40	Elisabeth Charlaix
	(to be updated)
09:40 to 10:00	Alberto Giacomello
	Liquids confined in nanopores
10:00 to 10:20	Hélène Berthoumieux
	Nonlocal dielectric response of water in nanoconfinement
10:20 to 10:40	Coffee break

Chair: Sabine Klapp

10:40 to 11:00	Pierre Illien
	Generalized correlation profiles in single-file diffusion
11:00 to 11:20	Christina Kurzthaler
	A geometric criterion for the optimal spreading of active polymers in porous media
11:20 to 11:40	Etienne Mangaud
	Chemisorbed vs physisorbed surface charge and its impact on electrokinetic transport: carbon vs boron nitride surface

11:40 to 12:00	Baptiste Coquinot Quantum interfacial phenomena in nanoscale water flows: unconventional friction and electric current generation
12:00 to 12:20	Thomas Franosch Structural relaxation in confined colloidal liquids within mode-coupling theory

Session: Charged systems

Chair: Luc Belloni

14:00 to 14:40	Roland Netz Generalized Langevin equation from a novel hybrid projection scheme and applications to protein folding
14:40 to 15:00	Iurii Chubak Quadrupolar NMR relaxation for ions in aqueous solutions from classical molecular dynamics
15:00 to 15:20	Yael Avni Conductivity of concentrated electrolytes
15:20 to 15:40	Coffee break

Chair: René van Roij

15:40 to 16:20	Stefano Sacanna Harnessing Coulombic forces to guide colloidal self-assembly
16:20 to 16:40	Thomas Leblé Recent results and old questions around Coulomb/Riesz systems from a mathematical perspective
16:40 to 17:00	Alina Ciach Correlation functions in concentrated electrolytes from combined density functional and statistical field theories
17:00 to 17:40	Susan Perkin Chemistry and complexity of interactions in natural electrolytes
17:40 to 19:00	Poster session
19:30 to 00:00	DINNER

Day 4 – Thursday, July 7th, 2022

Session: Soft matter (part II)

Chair: Jean-François Joanny

09:00 to 09:40	Ramin Golestanian
	Self-organization via non-reciprocal interactions
09:40 to 10:00	Alberto Dinelli
	Self-organization of bacterial mixtures interacting via quorum sensing
10:00 to 10:20	Joakim Stenhammar
	Osmotic stability and thermal fluctuations of giant unilamellar vesicles
10:20 to 10:40	Coffee break

Chair: Werner Krauth

10:40 to 11:00	Jure Dobnikar
	Self-assembly of viral capsids and packing of genome
11:00 to 11:20	Charlie Duclut
	Hydraulic and electric control of cell spheroids
11:20 to 11:40	Sophie Marbach
	The nanocaterpillar's random walk or how to move with jiggly and sticky feet
11:40 to 12:20	Joachim Dzubiella
	Structure and dynamics of models of (active) responsive colloids
12:20 to 12:40	Farewell from the Organizers

3. Abstracts – Talks

July 4th, 2022 (Monday)

14:50 to 15:30

Density depletion and enhanced fluctuations in ‘water’ near hydrophobic solutes: identifying the underlying physics

Robert Evans

University of Bristol, United Kingdom

The origin of the density depletion and enhanced density fluctuations that occur in water in the vicinity of an extended hydrophobic solute are investigated. We argue that both phenomena are remnants of the critical drying surface phase transition that occurs at liquid-vapour coexistence in the macroscopic planar limit, i.e., as the solute radius $R_s \rightarrow \infty$. Focusing on the density profile and a sensitive spatial measure of fluctuations, the local compressibility profile, we develop a scaling theory which expresses the extent of the density depletion and enhancement in compressibility in terms of R_s , the strength of solute-water attraction, and the deviation from liquid-vapor coexistence $\delta\mu$.

Testing the predictions against results of i) classical density functional theory for a simple (LJ) solvent and ii) grand canonical Monte Carlo simulations of a popular water model (mw), we find that the theory provides a firm physical basis for understanding how water behaves at a hydrophobe.

*Work with Mary K. Coe and Nigel B. Wilding

15:30 to 15:50

Noether's theorem in statistical mechanics

Sophie Hermann, Matthias Schmidt

University of Bayreuth, Germany

Noether's Theorem [1] is familiar to most physicists due its fundamental role in linking the existence of conservation laws to the underlying symmetries of a physical system. Typically the systems are described in the particle-based context of classical mechanics or on the basis of field theory. We apply Noether's calculus of invariant variations to thermal systems, where fluctuations are paramount and one aims for a statistical mechanical description, both in and out of equilibrium. Generating functionals, such as the free energy, yield mechanical laws under continuous translational and rotational symmetry operations. The resulting global theorems express vanishing of total internal and total external forces and torques. Local sum rules interrelate density correlators, as well as static and time direct correlation functions via infinite hierarchies, including memory. We demonstrate that this approach is consistent with the earlier work in equilibrium [2-4], and that it enables one to go, with relative ease, beyond the sum rules that these authors formulated. For anisotropic particles, systematic coupling of orbital and spin motion is identified. The theory allows to shed new light on the spatio-temporal coupling of correlations in complex systems. We present novel exact and nontrivial identities [5, 6] that apply to time-dependent problems and driven and active fluids [7, 8].

[1] E. Noether, Nachr. d. König. Gesellsch. d. Wiss. zu Göttingen, Math.-Phys. Klasse 235 (1918)

[2] R. Evans, Advances in Physics, **28**, 143-200 (1979)

[3] M. Baus, Molecular Physics, **51**, 211-220 (1984)

[4] J. P. Hansen and I. R. McDonald, 'Theory of Simple Liquids', Academic Press, London (2013)

[5] S. Hermann, M. Schmidt, Commun. Phys., **4**, 176 (2021)

[6] S. Hermann, M. Schmidt, J. Phys.: Condens. Matter, (2022)

[7] S. Hermann, P. Krinninger, D. de las Heras, M. Schmidt, Phys. Rev. E, **100**, 052604 (2019)

16:10 to 16:30

Thermal forces: from nanotubes to thermophoresis

Alberto Parola, Pietro Anzini, Zeno Filiberti
Universita' dell'Insubria, Italy

Fluid motion induced by thermal gradients is a well-known phenomenon with remarkable consequences, especially in rarefied gases (e.g. Crookes' radiometer). In the absence of external forces, thermal gradients in a fluid give rise to a non-equilibrium stationary state characterized by heat flux and no mass current. However, when the fluid is confined by a surface parallel to the gradient, a "thermal force" is generated, setting the fluid into motion. This effect, known as thermosmosis, plays a key role when fluids are confined in nanotubes, is relevant in understanding the pressure difference through a membrane separating two reservoirs at different temperatures and is the driving mechanism for thermophoresis in colloidal suspensions. The microscopic description of this non-equilibrium state can be consistently obtained by use of Linear Response Theory [1]. This analysis allows to identify the microscopic expression of the underlying "thermal force", to provide the generalization of the macroscopic Stokes equation in confined environments (like nanotubes) and to show how the viscosity coefficient is modified by the presence of a wall. Molecular Dynamics simulations of fluid flow in a thermal gradient and under confinement allow to study the resulting velocity profile extracting a useful scaling law for the pressure difference across the tube [2] paving the way to a microscopic understanding of particle thermophoresis.

[1] P. Anzini, G. Colombo, Z. Filiberti, A. Parola, Phys. Rev. Lett., **123**, 028002 (2019)

[2] P. Anzini, Z. Filiberti, A. Parola, Fluid flow at interfaces driven by thermal gradients (archive)

16:30 to 16:50

Toward a molecular picture of thermodiffusion of dilute aqueous solutions

Guillaume Stirnemann
CNRS Institut de Biologie Physico-Chimique, France

The emergence of life is one of the most fascinating and yet largely unsolved questions in the natural sciences, and thus a significant challenge for scientists from many disciplines. I will discuss our recent investigation of the poorly-understood thermally-driven process of thermophoresis, which was shown to be an efficient process for the accumulation of dilute precursors in the absence of biological compartments. I will show how our molecular simulations and calculations can shed light on the molecular mechanisms associated with thermodiffusion.

First, I will demonstrate that we can establish a robust simulation set-up to study this problem using non-equilibrium molecular dynamics simulations. I will then show that such simulations lead to results in very good agreement with available experimental data, and previous simulations on model mixtures. We will then see that theories and models that had been suggested in the literature cannot explain thermodiffusion in these solutions, and we will point toward the possible origins for this phenomenon.

Reactive mixture as a model for fluids with water-like anomalies**Frédéric Caupin¹**, Mikhail A. Anisimov¹Université Claude Bernard Lyon 1, France²University of Maryland, College Park, United States

Liquid polyamorphism is the possibility for a pure substance to exist in multiple liquid phases. Examples include water, phosphorous, and sulfur. To gain general insight into this phenomenon beyond each particular instance, we looked for a statistical physics model with minimal ingredients [1]. The compressible binary mixture on a lattice [2] provides such a model, once its two components are allowed to interconvert like in a chemical reaction, with associated changes in energy and entropy. Varying one interaction parameters allows generating various cases with and without liquid polyamorphism and various types of thermodynamic anomalies. An off-lattice version of this reactive mixture model is currently being developed.

[1] F. Caupin, M. Anisimov, Phys. Rev. Lett., **127**, 185701 (2021)[2] D. Furman, S. Dattagupta, R. Griffiths, Phys. Rev. B, **15**, 441-464 (1977)**Connection between water's dynamical and structural properties: insights from ab initio simulations.****Cecilia Herrero¹**, Michela Pauletti², Gabriele Tocci², Marcella Iannuzzi², Laurent Joly³¹Université de Montpellier, France²Department of Chemistry, University of Zurich, Switzerland³Institut Lumière Matière, Université Claude Bernard Lyon 1, France

Among all fluids, water has always been of special concern for scientists from a broad variety of research fields due to its rich behavior. In particular, some questions remain unanswered nowadays concerning the temperature dependence of bulk and interfacial transport properties of supercooled and liquid water, *e.g.* regarding the fundamentals of the violation of the Stokes-Einstein relation in the supercooled regime or the subtle relation between structure and dynamical properties. Here we used first-principle simulations (which explicitly solve the electronic structure) based on density functional theory (DFT) to investigate the diffusion coefficient and viscosity of water as a function of temperature, in both liquid and supercooled regimes, and to explore the connection between these dynamical properties with the local structure. In this work, we reported several important findings. From the technical and practical point of view, by comparing different frequently employed and more recent exchange-correlation functionals, we saw that the SCAN functional provides the best predictions of the dynamical properties, although they deteriorate at lower temperatures. From the fundamental point of view, our results clearly showed the validity of the Stokes-Einstein relation between the diffusion coefficient and the viscosity for all functionals, despite their different results for both properties, with a consistent hydrodynamic radius of 1 Angstrom across functionals. Furthermore, we observed that both dynamical properties satisfy scaling relations with the excess entropy (more precisely its 2-body approximation) computed solely from a simple structural property, namely the oxygen-oxygen radial distribution function. Beyond the physical implications of this observation in first-principles simulations of water (which confirms previous works on simpler fluids and with a simpler description of this complex fluid), this relation also suggests that the 2-body excess entropy can serve as a convenient proxy to gauge the ability of DFT or high accuracy methods to predict dynamical properties without actually computing them, thereby reducing significantly the required computational cost.

17:30 to 18:10

Structure and dynamics of interfacial water

Angelos Michaelides

University of Cambridge, United Kingdom

There are few molecules, if any, more important than water. However, remarkably little is known about how it interacts with surfaces, particularly at the molecular level. In this talk I will discuss some of our recent work on the application and development of a variety of state of the art computer simulation methods to better understand the structure and dynamics of water at surfaces and under confinement. Specific topics discussed will include work carried out in collaboration with experimentalists to understand the growth and diffusion of ice clusters at metal surfaces, heterogenous ice nucleation, and water confined within 1- and 2-dimensional membranes. Methodological developments aimed at providing more accurate treatments of adsorption on and bonding within solids will also be covered, as well as an efficient machine learning strategy for simulating complex aqueous interfaces.

July 5th, 2022 (Tuesday)

09:00 to 09:40

Phase transitions in the growth of bacterial biofilms

Rosalind Allen, Ellen Young, Gavin Melaugh

Friedrich Schiller University, Jena, Germany

Microorganisms such as bacteria are similar in size to colloidal particles but they show highly non-equilibrium behaviours such as swimming and proliferation. Focusing on proliferation, we use computer simulations to investigate the dynamics of bacterial biofilms: assemblies of bacteria that grow on surfaces. Depending on the parameters, we find different biofilm spatial structures and dynamics. We rationalise our findings in the form of a phase diagram for pinning of the biofilm interface. We also infer patterns of gain and loss of genetic diversity within our simulated biofilms, suggesting a connection between spatial structure and evolution within the biofilms.

09:40 to 10:00

Modeling and simulating charged patchy colloids

Emanuela Bianchi¹, Silvano Ferrari¹, Emanuele Locatelli²

¹Technische Universität Wien, Austria

²University of Padova, Italy

Heterogeneously charged colloids are promising building blocks for the self-assembly of target structures with specific properties at the nano- and micro-scale [1]. As the theoretical approach is straightforward but not trivial [2,3], we recently developed an open access tool to (i) calculate the electrostatic potentials for any surface charge distribution of the colloids, and (ii) build a coarse-grained model that – within well-defined limits – accurately reproduces the reference electrostatic potential [4]. While the proposed model can be reliably applied to heterogeneously charged colloids

with a charged equatorial belt and two oppositely charged poles, more complicated charge topologies might be faithfully described only by the full electrostatic approach. We thus investigate how the mismatch between the full electrostatic and the coarse-grained interaction energy changes according to the system parameters for two case studies that are both relevant for experiments: charged Janus colloids and charged particles with two non-polar patches [4]. Moreover, we test the effects of these possible mismatches on the assembly behavior by running Monte Carlo (MC) simulations of both case studies with either the electrostatic or the coarse-grained potential [4]. The coarse-grained model can be easily implemented in Molecular Dynamics (MD) simulations: we then explore the advantages and the limits of our coarse-grained model implementation [5].

[1] E. Bianchi, P.D.J. van Oostrum, C. Likos, G. Kahl, *Current Opinion in Colloid & Interface Science*, **30**, 18 (2017)

[2] Emanuela Bianchi, Gerhard Kahl and Christos N. Likos, *Soft Matter*, **7**, 8313 (2011)

[3] Monika Stipsitz, Gerhard Kahl and Emanuela Bianchi, *J.Chem. Phys.*, **142**, 114905 (2015)

[4] E. Locatelli and E. Bianchi, in preparation

[5] S. Ferrari, E. Locatelli, G. Kahl and E. Bianchi, in preparation

10:00 to 10:20

Why the world is simple: the algorithmic evolution of self-assembly

Ard Louis

Oxford University, United Kingdom

In the famous trope of monkeys typing at random on keyboards, the probability of typing a specific sequence of length L on a keyboard of N keys, is simply $1/N^L$. In this scenario, all outputs of length L are equally likely. Now consider the monkeys typing instead into a computer program. They might accidentally type, with probability $1/N^{20}$, the 20 character code "print "01" 500 times" which will output an ordered sequence of length $L=1000$ of the form 0101010.... In this second "algorithmic" scenario, outputs with short codes are much more likely to appear than others. This intuitive picture has been formalised in the coding theorem of algorithmic information theory (which should be much more widely taught to physicists!). It suggests that many processes in nature may be highly biased towards simple outputs, that is outputs with short effective programs. Evolution proceeds by random genetic mutations which are translated by developmental processes into biological outputs called phenotypes, so we should expect the second "algorithmic" scenario to hold. The coding theorem therefore predicts that random mutations in evolution are exponentially more likely to generate simpler, more compressible outputs. Evidence for this strong bias towards simplicity and symmetry has been found in self-assembling protein clusters, the structure of RNA, and in gene regulatory structures~[1,2]. It allows us to predict which phenotypes are found in nature. It can also be used to guide the design of artificial self-assembling nano-structures. These same principles predict an Occam's razor-like bias in deep neural networks~[3], suggesting an intriguing link between theories of learning and biological evolution.

[1] Johnston, K., Dingle, S., Greenbury, C., Camargo, J., Doye, S., Ahnert, A., Louis, A., Johnston et al. <https://doi.org/10.1101/2021.07.28.454038>

[2] K. Dingle et al, *J. Mol. Bio Evol.* <https://doi.org/10.1093/molbev/msab280>

[3] G. Valle Pérez et al, <https://arxiv.org/abs/1805.08522>

10:40 to 11:00

Colloidal active matter

Hartmut Löwen

Heinrich – Heine Universität Düsseldorf, Germany

Active particles which are self-propelled by converting energy into mechanical motion represent an expanding research realm in physics and chemistry and engineering. One of the key examples are self-propelled micron-sized colloidal Janus particles moving in a liquid (“microswimmers”). In a water-lutidine binary mixture close to the lower critical point laser illumination leads to wetting of one particle side by a lutidine-rich phase which brings about self-diffusiophoretic self-propulsion that can be steered by laser illumination. In this talk, several phenomena are described including motility-induced phase separation (MIPS) of active particles, motion of Janus particles in optical motility landscapes, and the formation of active colloidal molecules by bringing together two immotile building blocks [2]. Finally, we describe how surface wetting controls the formation of active dropoids which are moving droplets containing active colloidal particles as intrinsic motors [3].

[1] C. Bechinger, R. di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, G. Volpe, *Reviews of Modern Physics* **88**, 045006 (2016).

[2] F. Schmidt, B. Liebchen, H. Löwen, G. Volpe, Light-controlled assembly of active molecules, *J. Chem. Phys.* **150**, 094905 (2019).

[3] J. Grauer, F. Schmidt, J. Pineda, B. Midtvedt, H. Löwen, G. Volpe, B. Liebchen, Active dropoids, *Nature Communications* **12**, 6005 (2021).

11:00 to 11:20

Organisation of charged nano-platelets and their aggregates in liquids and gels

Natalie Malikova¹, Claire Hotton¹, Yasmine Sakhawoth¹, Anthony Beauvois², Laurent Michot¹, Pierre Levitz¹

¹Laboratoire de Physico-chimie des Electrolytes et des Nanosystèmes interfaciaux (PHENIX), Sorbonne Université, CNRS, France

²Synchrotron SOLEIL, l'Orme des merisiers, Saint-Aubin, Gif-sur-Yvette, France

Clay nanoparticles, main constituents of soil, occupy a very specific place in colloidal science: these negatively charged particles have a *plate-like* form. Shape anisotropy leads to a much richer phase diagram and to a more involved experimental and theoretical treatment of these systems. We have explored several aspects of clay organisation and their aggregation in both aqueous suspensions and in water-based gels (hydrogels).

Concerning clay suspensions, we studied clay aggregation by ionenes, a class of cationic polyelectrolytes with a regular charge density, which can be tuned to match/mismatch the clay charge density. The multi-scale structure of these clay-polyelectrolyte aggregates is determined by a combination of small angle X-ray scattering (SAXS) and scanning transmission X-ray microscopy (STXM). Locally, we see clear evidence for the formation of clay tactoids (dense face-to-face platelet organisation), within the otherwise loose aggregates. The relative charge density of the polyelectrolyte chains and clay surfaces is a key parameter for the repeat distance within these tactoids (of the order of 1nm), but also tactoid abundance and possibly even the macroscopic aggregate density [1]. The extent of stacking (5–10 platelets per tactoid) is a general feature of all the systems, and its origin remains unknown. Very special features are observed in the process of polyelectrolyte-induced clay aggregation starting with clay suspensions with multivalent atomic counterions, such as Ca^{2+} and La^{3+} . In such cases, an equilibrium is established between two types of tactoids, those held together purely by multivalent atomic ions on one hand and by polyelectrolyte chains on the other. Surprisingly, no “mixed” tactoids are observed.

The face-to-face organisation of clay platelets is equally reproduced in ionene-based hydrogels, albeit at much larger clay separations (tens of nm), which is decided by the underlying mesh size of the polyelectrolyte hydrogel network [2]. Interestingly, the degree of nanoplatelet ordering in the hydrogel is very sensitive to the negative charge location on the clay platelet. Increased nanoplatelet ordering leads to an improvement of the elastic properties of the hydrogel. On the contrary, the presence of dense clay aggregates (tactoids), induced by multi-valent clay counterions, destroys the

hydrogel network. We are currently exploring the possibility of a unique nanoplatelet orientation inside the hydrogel (application of a magnetic field), in order to yield a versatile system with potentially anisotropic permeability properties.

[1] Y. Sakhawoth, L. Michot, P. Levitz, A.-L. Rollet, J. Sirieix-Plenet, D. Hermida Merino and N. Malikova, *Langmuir* **35**, 10937-10946 (2019).

[2] C. Hotton, J. Sirieix-Plenet, G. Ducouret, T. Bizien, A. Chenneviere, L. Porcar, L. Michot and N. Malikova, *J. Colloid and Interface Science* **604**, 2021, 358-367, 10.1016/j.jcis.2021.07.010

11:20 to 11:40

Cahn-Hilliard theory for capacitive diffusion in colloidal fluids

Michiel Sprik

University of Cambridge, United Kingdom

What will happen if diffusion in colloidal fluids can store energy in addition to dissipating it? This question is investigated applying a Cahn-Hilliard scheme in which the fluctuation of the density is represented as the divergence of a hypothetical mass polarization field. The energy cost of polarization is modeled by extending the free energy density with the square of the polarization divided by a susceptibility. This in general non-linear functional is simplified to quadratic form by approximating the density dependent term as a square of the density fluctuations yielding a square divergence model for polarization. In agreement with the related square density gradient model, the Gaussian density fluctuations decay exponentially with distance. The characteristic length is proportional to the square root of the susceptibility. Contrary to the square density gradient model, the long wave length density fluctuations are fully suppressed. The structure factor vanishes for $k=0$. This is the hallmark of hyperuniformity [1]. The implication for the relaxation is investigated in the framework of the conserved gradient flow scheme of Cahn-Hilliard theory. The results confirm that the dynamical process can be viewed as a form of capacitive diffusion. The phenomenology of the long wave length static correlations is however very similar to the one-component plasma. We end the talk therefore with a quick comparison to this classic example of hyperuniformity reformulating the electrostatics in a pseudo-dielectric representation as previously applied to the Poisson-Boltzmann theory of ionic solutions [2].

[1] S. Torquato, F. Stillinger, *Phys. Rev. E*, **68**, 041113 (2003)

[2] M. Sprik, *Phys. Rev. E*, **103**, 022803 (2021)

11:40 to 12:20

From theory of simple liquids to machine learning

Marjolein Dijkstra

Utrecht University, Netherlands

Jean-Pierre Hansen has been highly influential in theory and simulations of simple and complex liquids. Predicting the emergent properties of soft matter from a microscopic description is a scientific challenge. In recent years, machine learning and reverse-engineering have opened new paradigms in the understanding and design of materials, next to theory and simulations. However, the soft-matter field has lagged far behind in embracing this approach for materials design. The main difficulty stems from the importance of entropy, the ubiquity of multi-scale and many-body interactions, and the prevalence of non-equilibrium and active matter systems. The abundance of exotic soft-matter phases with (partial) orientation and positional order like liquid crystals, quasicrystals, plastic crystals, along with the omnipresent thermal noise, makes the classification of these states of matter using ML tools highly non-trivial. In this talk, I will address questions like: Can we use machine

learning to autonomously identify local structures [1], detect phase transitions, classify phases and find the corresponding order parameters [2] in soft-matter systems, can we identify the kinetic pathways for phase transformations [3], and can we use machine learning to coarse-grain our models [4]? Finally, I will show how one can use machine learning to reverse-engineer the particle interactions to stabilize nature's impossible phase of matter, namely quasicrystals [5]?

[1] J.E. Boattini, M. Dijkstra, L. Fillion, J. Chem. Phys., **151**, 154901 (2019)

[2] R. van Damme, G. Coli, R. van Roij, M. Dijkstra, ACS Nano, **14**, 15144-15153 (2020)

[3] G. Coli, M. Dijkstra, ACS Nano, **15**, 4335-4346 (2021)

[4] G. Campos-Villalobos, E. Boattini, L. Fillion, M. Dijkstra, J. Chem. Phys., **155**, 174902 (2021)

[5] G. Coli, E. Boattini, L. Fillion, M. Dijkstra, Sci. Adv., **8**, (2022)

14:00 to 14:40

Computer simulations of glassy liquids: what are the new frontiers?

Ludovic Berthier

CNRS, France

Jean-Pierre Hansen performed pioneering work to demonstrate that Molecular Dynamics simulations can give unique insights into the microscopic behavior of dense liquids approaching the glass transition. Combining this approach to smart Monte Carlo techniques, it is now possible to generate equilibrium configurations of deeply supercooled liquids at all experimentally-relevant temperatures. These recent developments have allowed a full exploration of thermodynamic properties and putative equilibrium phase transitions underlying the formation of glasses. This improved knowledge also informs studies of the microscopic dynamics of dense liquids near the glass transition. I will summarise the current state of the art of the field, and describe the challenges ahead of us.

14:40 to 15:00

Imaging and quantifying strongly confined flow of fat crystal dispersions with rheo-MRI

Klaudia Milc, Joshua Dijksman, John van Duynhoven, Camilla Terenzi

Wageningen University and Research, Netherlands

Flow of complex dispersions, with particle sizes not much smaller than the flow geometries used, occurs in many industrial and everyday-life situations. In the production of foods or cosmetics, which typically feature micron-sized particles, fluids are extruded through mm-sized nozzles into molds, while during customer use the products are spread into μm -thin layers. It is now well established that, under such strongly confined conditions, flow of particulate dispersions can become cooperative. As a result of cooperativity effects, the flowing material is macroscopically fluidized and, thus, exhibits enhanced velocities and higher spatial heterogeneities of viscosity as compared to theoretical predictions in the absence of cooperativity. Accounting for, and quantifying, flow cooperativity in optically-opaque dispersions still remains an unsolved challenge in fundamental studies and industrial applications, due to lack of comprehensive velocimetry data, acquired with high spatial resolution, and lack of rheological models suitable for a range of confined flow geometries.

To resolve cooperativity in opaque materials, we use a novel sub-mm rheo-MRI setup to identify and study flow cooperativity in a food precursor, fat crystal dispersions (FCDs), upon varying the crystallization conditions. By varying the crystallization conditions, we alter the multiscale microstructure of the FCDs, which ranges from the nanometer-sized platelets, and the dispersed

fractal aggregates, up to the meso-scale of the weak-link network. We introduce a numerical fitting method, based on the fluidity model, which yields the cooperativity length in the narrow-gap CC. Thanks to the high-resolution local velocimetry data, and a versatile theoretical approach, we show that flow cooperativity emerges only in the FCDs with aggregates sizes smaller than the confinement size by at least an order of magnitude. We attribute this result to the correspondingly increased mobility of the aggregates, absent at larger particle sizes. We foresee that our proposed combination of high-resolution narrow-gap rheo-MRI measurements and numerical fitting analysis approach will propel further similar flow studies of other multi-scale and optically-opaque materials.

15:00 to 15:20

Unraveling structural and dynamical features in glassy fluids using machine learning

Laura Filion

Debye Institute for Nanomaterials Science, Utrecht University, Netherlands

Developments in machine learning (ML) have opened the door to fully new methods for studying phase transitions due to their ability to extremely efficiently identify complex patterns in systems of many particles. Applications of machine learning techniques vary from the use of developing new ML-based order parameters for complex crystal structures, to locating phase transitions, to speeding up simulations. The rapid emergence of multiple applications of machine learning to statistical mechanics and materials science demonstrates that these techniques are destined to become an important tool for soft matter physics. In this talk, I will briefly present an overview of the work my group is doing on using ML to study soft matter systems, with a focus on a new strategy to fit the dynamics in glassy systems using advanced hierarchical order parameters combined with simple linear regression [1]. Additionally, I will present a new method for extracting the cage structure of a glassy configuration, and demonstrate that this information significantly improves our ability to predict both short-time and long-time glassy dynamics.

[1] E. Boattini, F. Smallegange, L. Filion, Phys. Rev. Lett., **127**, 088007 (2021)

15:40 to 16:00

Overlap and glass quantization of the Gaussian core model

Jean-Marc Bomont¹, Christos Likos², Jean-Pierre Hansen³

¹University of Lorraine, France

²Faculty of Physics, University of Vienna, Austria

³CNRS and Sorbonne Université, Laboratoire PHENIX, France

Systems of ultrasoft particles exhibit complex liquid-solid phase diagrams. In order to study the dynamical glass transition occurring within these systems, we use the replica method, involving two identical copies, conjugated with classical integral equation theories of the liquid state, focusing on low temperatures and low-to-moderate densities. For particles interacting through the Gaussian Core Model, we demonstrate that at constant temperature, a "continuous" glass state is entered upon a first compression but this glass melts as the density is further increased. In addition to this reentrant transition, a second, transition is discovered at higher densities between the "continuous" glass and a quantized glass. The overlap Q (i.e. the order parameter of the transition) of the former is

a continuous function of temperature, while Q of the latter exhibits a succession of stripes. The glass physics of ultrasoft particles is hence richer than that of impenetrable particles.

16:00 to 16:40

How amorphous materials yield under stress: a new kind of out of equilibrium phase transition

Giulio Biroli

ENS Paris

I will show that a new kind of out of equilibrium phase transition is at the core of how amorphous solids yield in response to external deformations—a phenomenon that is crucial both for practical applications and for theoretical reasons. Such phase transition has strong connections with phenomena studied in the theory of disordered systems such as the zero-temperature spinodal of the Random Field Ising Model, the Depinning transition, and rare events.

Our results unveil that despite large differences in the materials' microscopic interactions and typical scales (from colloids to molecular glasses) a large degree of universality emerges as there are only two ways in which amorphous solids respond to a deformation: One, typical of well-annealed materials, is characterized by an abrupt failure with a macroscopic stress drop and the sudden emergence of sharp shear bands ; the other, typical of poorly annealed materials, shows merely a smooth crossover. By varying the preparation protocol, one can change the response of a given material from one to the other, and this change is controlled by a random critical point, akin to the one of the zero temperature Random Field Ising Model. We will confirm our scenario by molecular dynamics simulations, and by analytical and numerical analysis of elastoplastic models.

16:40 to 16:50

The European Physical Journals – From scientists for scientists

Roland Netz

Free University of Berlin, Germany

16:50 to 17:10

Life in the abyss: the hydro-structural connection

Sauro Succi

Italian Institute of Technology, Italy

Since its discovery, the deep-sea glass sponge *Euplectella aspergillum* has attracted interest on account of its amazing mechanical properties and sheer beauty. Its skeletal system consists of amorphous hydrated silica and is arranged in a highly regular and hierarchical cylindrical lattice that begets exceptional flexibility and resilience to damage. Structural analyses dominate the literature, while hydrodynamic fields that surround and penetrate the sponge have remained largely

unexplored. Here we address the question as to whether, besides improving its mechanical properties, the skeletal motifs of *E. aspergillum* underlie the optimization of the flow physics within and beyond its body cavity.

To this purpose, we use large-scale lattice Boltzmann simulations, featuring over fifty billion grid points and spanning over three spatial decades [1]. These *in silico* experiments indicate that the skeletal motifs reduce the overall hydrodynamic stress and support coherent internal recirculation patterns at low flow velocity. These hydro-structural patterns are arguably beneficial to the organism for selective filter feeding and sexual reproduction. The present study reveals mechanisms of extraordinary adaptation to live in the abyss, paving the way towards further studies of this type at the intersection between fluid dynamics, structural mechanics and functional ecology.

[1] G. Falcucci, G. Amati, P. Fanelli, V. Krastev, G. Polverino, M. Porfiri, S. Succi, *Nature*, 595, 537-541 (2021)

July 6th, 2022 (Wednesday)

09:00 to 09:40

Title (to be updated)

Elisabeth Charlaix

LiPhy, Université Joseph Fournier, Grenoble, France

09:40 to 10:00

Liquids confined in nanopores

Alberto Giacomello

Sapienza University of Rome, Italy

In nanopores, the phase behavior of liquids is dramatically altered; there, the extreme confinement and hydrophobicity concur to the formation of nanoscale bubbles – drying. While this process is known to occur in solid-state nanopores [1], the hydrophobicity of the cavity of several biological ion channels may also lead to drying [2,3]. Such bubbles, in turn, impede the passage of ions which require a solvation shell to translocate through the pore; this mechanism – the so-called hydrophobic gating – thus effectively blocks ion currents. In this talk, the thermodynamics and kinetics of drying are discussed in the light of recent results based on theory and simulations, clarifying the effect of hydrophobicity, geometry, size, and connectivity of nanopores [4]. The emergence of nanoscale effects not accounted for in macroscopic theories is considered together with the open challenges in simulating such systems. In particular, the presence of small concentrations of dissolved gases in solution is found to accelerate the drying process [5]. The relevance of the reported exotic behaviour of liquids confined in nanopores is discussed in the realm of biomimetic nanopore devices and of general anesthesia.

[1] A. Tinti, A. Giacomello, Y. Grosu, C. Casciola, *Proc. Natl. Acad. Sci. USA.*, **114**, E10266-E10273 (2017)

[2] R. Roth, D. Gillespie, W. Nonner, R. Eisenberg, *Biophysical Journal*, **94**, 4282-4298 (2008)

[3] C. Guardiani, D. Sun, A. Giacomello, *Front. Mol. Biosci.*, **8**, (2021)

[4] A. Giacomello, R. Roth, *Advances in Physics: X*, **5**, 1817780 (2020)

[5] G. Camisasca, A. Tinti, A. Giacomello, *J. Phys. Chem. Lett.*, **11**, 9171-9177 (2020)

Nonlocal dielectric response of water in nanoconfinement

Hélène Berthoumieux¹, Geoffrey Monnet², Fernando Bresme³, Alexei Kornyshev³

¹Sorbonne Science Université, France

²ENS, France

³Imperial College, United Kingdom

Recent experiments reporting a very low dielectric permittivity for nanoconfined water have renewed the interest to the structure and dielectric properties of water in narrow gaps [1]. In this work, a nanometric water slab confined between graphene or boron nitride surfaces is described with a minimal Landau-Ginzburg field-theory composed of a nonlocal bulk-determined term and a local water-surface interaction term [2]. This model allows to show how the interplay between the boundary conditions and the intrinsic bulk correlations of the fluid encodes dielectric properties of confined water. This theoretical analysis is supported and validated by molecular dynamics simulations and comparison with the experimental data.

[1] L. Fumagalli, A. Esfandiar, R. Fabregas, S. Hu, P. Ares, A. Janardanan, Q. Yang, B. Radha, T. Taniguchi, K. Watanabe, G. Gomila, K. Novoselov, A. Geim, *Science*, **360**, 1339-1342 (2018)

[2] G. Monet, H. Berthoumieux, F. Bresme, A. Kornyshev, *Phys. Rev. Lett.*, **126**, 216001 (2021)

10:40 to 11:00 Coffee break

Generalized correlation profiles in single-file diffusion

Pierre Illien

CNRS, Sorbonne Université, France

Single-file transport, where particles diffuse in narrow channels while not overtaking each other, is a fundamental model for the tracer subdiffusion observed in confined systems, such as zeolites or carbon nanotubes. Most approaches to this celebrated many-body problem were restricted to the description of the tracer only. Here, we go beyond this standard description by introducing and providing analytical results for generalized correlation profiles in the frame of the tracer. In addition to controlling the statistical properties of the tracer, these quantities fully characterise the correlations between the tracer position and the density of bath particles. Considering the hydrodynamic limit of the problem, we determine the scaling form of the correlation profiles with space and time, and unveil a non-monotonic dependence with the distance to the tracer despite the absence of any asymmetry. Our analytical approach provides several exact results for the generalized correlation profiles for several paradigmatic models of single-file diffusion. Among them, we consider in particular the symmetric exclusion process, for which we find an exact closed equation satisfied by the correlations, therefore breaking the hierarchy of equations that arises from the many-body nature of the problem.s:

1. A. Poncet, A. Grabsch, P. Illien, O. Bénichou, *Phys. Rev. Lett.* **127**, 220601 (2021). arXiv:2103.13083.

2. A. Grabsch, A. Poncet, P. Rizkallah, P. Illien, O. Bénichou, to appear in *Science Advances*, arXiv:2110.09269.

11:00 to 11:20

A geometric criterion for the optimal spreading of active polymers in porous media

Christina Kurzthaler¹, Suvendu Mandal², Tapomoy Bhattacharjee³, Hartmut Löwen⁴, Sujit S. Datta¹, Howard A. Stone¹

¹Princeton University, United States

²Technische Universität Darmstadt, Germany

³Tata Institute of Fundamental Research, Bangalore, India

⁴Heinrich-Heine-Universität Düsseldorf, Germany

Efficient navigation through disordered, porous environments poses a major challenge for swimming microorganisms and future synthetic cargo-carriers. We perform Brownian dynamics simulations of active stiff polymers undergoing run-reverse dynamics, and so mimic bacterial swimming, in porous media. In accord with experiments of *Escherichia coli*, the polymer dynamics are characterized by trapping phases interrupted by directed hopping motion through the pores. Our findings show that the spreading of active agents in porous media can be optimized by tuning their run lengths, which we rationalize using a coarse-grained model. More significantly, we discover a geometric criterion for the optimal spreading, which emerges when their run lengths are comparable to the longest straight path available in the porous medium. Our criterion unifies results for porous media with disparate pore sizes and shapes and for run-and-tumble polymers. It thus provides a fundamental principle for optimal transport of active agents in densely-packed biological and environmental settings.

[1] C. Kurzthaler, S. Mandal, T. Bhattacharjee, H. Löwen, S. Datta, H. Stone, Nat. Commun., **12**, 7088 (2021)

11:20 to 11:40

Chemisorbed vs physisorbed surface charge and its impact on electrokinetic transport: carbon vs boron nitride surface

Etienne Mangaud¹, Marie-Laure Bocquet², Lydéric Bocquet³, Benjamin Rotenberg⁴

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²PASTEUR, Département de chimie, École normale supérieure, PSL University, Sorbonne Université, CNRS, Paris, France

³Laboratoire de Physique de l'Ecole normale Supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université de Paris, Paris, France

⁴Sorbonne Université, CNRS, Physicochimie des électrolytes et Nanosystèmes Interfaciaux, Paris, France

The possibility of controlling electrokinetic transport through carbon and hexagonal boron nitride (hBN) nanotubes has recently opened new avenues for nanofluidic approaches to face outstanding challenges such as energy production and conversion or water desalination [1]. The pH-dependence of experimental transport coefficients points to the sorption of hydroxide ions as the microscopic origin of the surface charge and recent *ab initio* calculations [2] suggest that these ions behave differently on carbon and hBN, with only physisorption on the former and both physisorption and chemisorption on the latter. Using classical non-equilibrium molecular dynamics simulations of interfaces between an aqueous electrolyte and three models of hBN and graphite surfaces, we demonstrate the major influence of the sorption mode of hydroxide ions on the interfacial transport properties [3]. Physisorbed surface charge leads to a considerable enhancement of the surface conductivity as compared to its chemisorbed counterpart, while values of the ζ -potential are less

affected. The analysis of the MD results for the surface conductivity and ζ -potential in the framework of Poisson–Boltzmann–Stokes theory[4], as is usually done to analyze experimental data, further confirms the importance of taking into account both the mobility of surface hydroxide ions and the decrease in the slip length with increasing titratable surface charge density.

- [1] S. Marbach, L. Bocquet, Chem. Soc. Rev., **48**, 3102-3144 (2019)
- [2] B. Grosjean, M. Bocquet, R. Vuilleumier, Nat. Commun., **10**, 1656 (2019)
- [3] E. Mangaud, M. Bocquet, L. Bocquet, B. Rotenberg, J. Chem. Phys., **156**, 044703 (2022)
- [4] T. Mouterde, L. Bocquet, Eur. Phys. J. E, **41**, 148 (2018)

11:40 to 12:00

Quantum interfacial phenomena in nanoscale water flows: unconventional friction and electric current generation

Baptiste Coquinot¹, Lydéric Bocquet¹, Nikita Kavokine²

¹LPENS, France

²Flatiron Institute, United States

Quantum effects are scarce in soft matter systems, where the dynamics are typically described using some version of Newton's equations. Yet, as the study of water flows is pushed to smaller and smaller scales, there appear phenomena that defy understanding in terms of classical theories of fluid transport. In particular, there is growing evidence for the coupling between fluid flows at the nanoscale and the electronic properties of the confining walls, resulting in both unconventional friction [1] and generation of electric currents inside the wall material [2]. In this talk, I will present some of our latest work on such quantum interfacial dynamics. Starting from the pioneering theoretical work on quantum friction [3], I will discuss the remarkable features of this phenomenon when water flows are confined down to the angström scale. I will then show how the framework of friction is generalized to account for current generation through two possible mechanisms: a Coulomb interaction between the fluid and the electrons of the solid and a viscous friction generating phonons which interact with the electrons [4]. In particular, we will show that it is possible to generate enormous currents, larger than expected by the literature, by choosing the right solid. Finally, I will discuss the favorable comparison between our theoretical predictions and recent experimental data.

- [1] E. Secchi, S. Marbach, A. Niguès, D. Stein, A. Siria, L. Bocquet, Nature, **537**, 210-213 (2016)
- [2] S. Ghosh, A. Sood, N. Kumar, Science, **299**, 1042-1044 (2003)
- [3] N. Kavokine, M. Bocquet, L. Bocquet, Nature, **602**, 84-90 (2022)
- [4] P. Král, M. Shapiro, Phys. Rev. Lett., **86**, 131-134 (2001)

12:00 to 12:20

Structural relaxation in confined colloidal liquids within mode-coupling theory

Thomas Franosch¹, Michele Caraglio¹, Lukas Schrack¹, Gerhard Jung², Charlotte F. Petersen³

¹University of Innsbruck, Austria

²Université de Montpellier, France

³The University of Sydney, Australia

The mode-coupling theory (MCT) of confined liquids [1] predicts multiple reentrant liquid-glass transitions which have been confirmed qualitatively in event-driven molecular dynamics simulations [2]. While the nonequilibrium state diagram and the nonergodicity parameters can be calculated numerically straight forwardly, the numerical implementation of the full time-dependence has

remained a challenge due to the new mathematical structure of the underlying equations. Only recently, we solved these numerical challenges and were able to provide a thorough investigation into the competing effects on the evolution of the structural relaxation [3]. In particular, we generalized and validated the beta-scaling of the glass transition to the case of multiple decay channels [4]. To disentangle the effects of confinement and layering we developed the concept of quasi-confinement where the hard walls are replaced by periodic boundary conditions with a period comparable to the particle diameter [5,6]. Numerical results and simulation confirm that the scenario of a multiple reentrant transition persists to these systems, yet the effects of confinement in slit geometry are much stronger suggesting that layering is the most important ingredient.

- [1] S. Lang, V. Botan, M. Oettel, D. Hajnal, T. Franosch, and R. Schilling, *Phys. Rev. Lett.* **105**, 125701 (2010).
 [2] S. Mandal, S. Lang, M. Gross, M. Oettel, D. Raabe, T. Franosch, and F. Varnik *Nat. Commun.* **5**, 4435 (2014).
 [3] G. Jung, M. Caraglio, L. Schrack, T. Franosch, *Phys. Rev. E* **102**, 012612 (2020)
 [4] G. Jung, Th. Voigtmann, T. Franosch, *J. Stat. Mech.* 073301 (2020)
 [5] L. Schrack, C. F. Petersen, G. Jung, M. Caraglio, T. Franosch *J. Stat. Mech.* 093301 (2020)
 [6] L. Schrack, C.F. Petersen, M. Caraglio, G. Jung, T. Franosch, *Journal of Statistical Mechanics: Theory and Experiment*, 043301 (2021)

14:00 to 14:40

Generalized Langevin equation from a novel hybrid projection scheme and applications to protein folding

Roland Netz, Cihan Ayaz
 Free University of Berlin, Germany

A novel hybrid projection scheme is introduced that combines linear Mori projection and conditional Zwanzig projection and used to derive a Generalized Langevin Equation (GLE) for a general interacting many-body system. The hybrid projection scheme allows to extract the GLE parameters from time series data in a form that is convenient for analytic and numerical treatment. Interestingly, memory effects can accelerate or slow-down barrier crossing: for intermediate memory decay times barrier crossing accelerates, while for long memory decay times, the barrier-crossing time increases with the memory time as a power law, which starkly violates the assumption of time-scale separation.

Protein-folding kinetics is often described as Markovian (i.e., memoryless) diffusion in a one-dimensional free energy landscape, governed by an instantaneous friction coefficient that is fitted to reproduce experimental or simulated folding times. For a few different examples, it is demonstrated that the friction extracted from molecular dynamics simulations exhibits significant memory with a decay time that is of the same order as the folding and unfolding times. Non-Markovian modeling not only reproduces the molecular dynamics simulations accurately but also demonstrates that memory friction effects lead to anomalous and drastically modified protein kinetics.

- [1] Cihan Ayaz, Lucas Tepper, Florian N. Brünig, Julian Kappler, Jan O. Daldrop, and Roland R. Netz, *PNAS* 2021 Vol. 118 No. 31 e2023856118

14:40 to 15:00

Quadrupolar NMR relaxation for ions in aqueous solutions from classical molecular dynamics

Iurii Chubak, Benjamin Rotenberg
 Sorbonne University, France

In nuclear magnetic resonance (NMR) experiments, the ions whose nuclei have spin $I > 1/2$ predominantly relax through the quadrupolar mechanism involving the interaction between the quadrupolar moment of the nucleus with the electric field gradient (EFG) at its position. While such experiments can potentially provide access to the structure, dynamics, and collective processes in ionic solvation shells, the amount of useful information that can be extracted in practice is often limited, as the quadrupolar coupling constant (QCC) that allows relating the measured NMR relaxation rate with a microscopic correlation time of EFG fluctuations are typically unknown. Both for aqueous ions at infinite dilution and in concentrated electrolytes, we show that a combination of classical molecular dynamics to sample long-time EFG fluctuations at the ion position with the consistently computed QCC at the ab initio level allows reaching a good agreement between the calculated and experimentally measured NMR rates [1, 2]. For ^{23}Na in aqueous NaCl, we find that the increase of the NMR rates with increasing the salt concentration or decreasing temperature is mainly due to the slow down of EFG fluctuations, whereas the effect of the QCC change is marginal [2]. We show that the correlation times of EFG fluctuations (~ 1 ps) are inconsistent with the correlation time of collective hydration shell rotations (~ 10 ps), a mechanism that is often used for rationalizing the quadrupolar NMR relaxation. In fact, our results suggest that collective symmetry-breaking effects in the first two hydration shells around the ion provide a microscopic pathway for the relaxation.

[1] I. Chubak, L. Scalfi, A. Carof, B. Rotenberg, J. Chem. Theory Comput., **17**, 6006-6017 (2021)

[2] I. Chubak, L. Alon, E. V. Silletta, G. Madelin, A. Jerschow, and B. Rotenberg, manuscript in preparation (2022).

15:00 to 15:20

Conductivity of concentrated electrolytes

Yael Avni¹, Ram Adar², David Andelman¹, Henri Orland³

¹Tel Aviv University, Israel

²College de France, France

³Institut de Physique Theorique, Université de Paris-Saclay, France

The conductivity of ionic solutions is arguably their most important trait, being widely used in electrochemical, biochemical, and environmental applications. The Debye-Hückel-Onsager theory successfully predicts the conductivity at very low ionic concentrations of up to a few millimolars, but there is no well-established theory applicable at higher concentrations. We study the conductivity of ionic solutions using a stochastic density functional theory, paired with a modified Coulomb interaction that accounts for the hard-core repulsion between the ions. The modified potential suppresses unphysical, short-range electrostatic interactions, which are present in the Debye-Hückel-Onsager theory. Our results for the conductivity show very good agreement with experimental data up to 3 molars, without any fit parameters. We provide a compact expression for the conductivity, accompanied by a simple analytical approximation.

[1] Y. Avni, R.M. Adar, D. Andelman and H. Orland, Phys. Rev. Lett. (in press, 2022)

15:40 to 16:20

Harnessing Coulombic forces to guide colloidal self-assembly

Stefano Sacanna¹, Shihao Zang¹, Theodore Hueckel¹, Glen Hocky¹, Jeremie Palacci²

¹New York University, United States

²UCSD, United States

From snowflakes to nanoparticle superlattices, a menagerie of complex structures emerge from simple building blocks attracting each other with Coulombic forces. On the colloidal scale, however, this self-assembly feat is not easily accomplished. Although many colloids bear an innate surface charge, their strong electrostatic attraction is not directly suitable for crystallization. Instead, particles must be finely crafted to serve as self-assembling units. In this talk, I'll show the robust assembly of crystalline materials from common suspensions of oppositely charged colloids through a generic approach which we refer to as polymer-attenuated Coulombic self-assembly. I will demonstrate that, when particles are held separated at specific distances by a neutral polymer spacer, the attractive overlap between oppositely charged electrical double layers can be systematically tuned, directing particles to disperse, crystallize, or become permanently fixed on demand.

16:20 to 16:40

Recent results and old questions around Coulomb/Riesz systems from a mathematical perspective

Thomas Leblé¹, Jeanne Boursier²

¹CNRS - Université de Paris, France

²Université Paris-Dauphine, France

The study of statistical mechanics systems involving long-range Coulomb or Riesz interactions has attracted considerable interest within the mathematical physics community in the last decade, notably around a line of work initiated by Sylvia Serfaty (see e.g. her plenary talk at the ICM 2018 - <https://arxiv.org/abs/1712.04095>). A big motivation (and some inspiration) came from trying to understand in a mathematical way the conjectures and results found in the physics/chemistry literature.

We thought it could be interesting to present some of the recent results obtained within the mathematical community around those topics, as well as the limitation of the present methods compared to physical arguments, and to take the opportunity to ask the experts on the “chimie physique” side for explanations, thoughts, and perhaps guidance!

16:40 to 17:00

Correlation functions in concentrated electrolytes from combined density functional and statistical field theories

Alina Ciach

Institute of Physical Chemistry of the Polish Academy of Sciences, Poland

Experiments show anomalous increase of correlations with increasing concentration of ions in concentrated electrolytes, whereas classical theories predict decreasing screening length. In the talk, a self-consistent theory for concentrated electrolytes will be presented. In our theory, oscillatory decay of the charge-charge correlation function with the decay length that shows perfect agreement with the experimentally discovered and so far unexplained scaling is obtained. For the density-density correlations, monotonic asymptotic decay with the decay length comparable with the decay length of the charge correlations is found. From the theory it follows that the correlation lengths in concentrated electrolytes depend crucially on the local variance of the charge density.

[1] A. Ciach, O. Patsahan, J. Phys.: Condens. Matter, **33**, 37LT01 (2021)

17:00 to 17:40

Chemistry and complexity of interactions in natural electrolytes

Susan Perkin¹, James Hallett², Timothy Groves¹, Kieran Agg¹

¹Oxford University, United Kingdom

²University of Reading, United Kingdom

Electrolytes are the 'background scenery' of cellular life, facilitating the interactions between proteins, nucleic acids, lipids, saccharides... all macromolecular assemblies. Although electrolytes are often simply characterised by a few generic parameters (ionic strength, permittivity), it is known that subtleties of their chemistry are crucial (as embodied in the Hoffmeister series) and non-ionic osmolytes also play a role. Recently emerging new insights into the two-way evolution of osmolyte/electrolyte composition and protein charge and structure gives a hint of further complexity.

In this talk I will report our initial explorations, involving simplistic model experiments, of the interaction between charged bodies across two classes of electrolyte: First, aqueous solutions of potassium chloride (KCl) and trimethylglycine ($\text{Me}_3\text{N}^+\text{CH}_2\text{COO}^-$, "TMG", a naturally occurring zwitterionic osmolyte) and second, aqueous solutions of guanidinium chloride ($\text{C}(\text{NH}_2)_3^+.\text{Cl}^-$, "Gdm.Cl"), a commonly employed protein denaturant.

Our emerging picture is one of subtle ion-specific effects, and collective interactions involving multiple components. On the horizon is the opportunity to tune screening, surface charge, and osmotic pressure independently through selection of an appropriate osmolytic recipe. Indeed, it appears that natural systems have taken full advantage of this fact to optimise function under diverse external influences (temperature, water chemical potential) for billions of years.

July 7th, 2022 (Thursday)

09:00 to 09:40

Self-organization via non-reciprocal interactions

Ramin Golestanian

Max Planck Institute for Dynamics and Self-Organization, Germany

I will discuss a generic mechanism by which such chemically-active particles, be it cells or enzymes or engineered synthetic colloids, can "sense" each other and ultimately self-organize in a multitude of ways. A peculiarity of these chemical-mediated interactions is that they break action-reaction symmetry: for example, one particle may be repelled from a second particle, which is in turn attracted to the first one, so that it ends up "chasing" it. Such chasing interactions allow for the formation of large clusters of particles that "swim" autonomously. Regarding enzymes, we find that they can spontaneously aggregate into clusters with precisely the right composition, so that the product of one enzyme is passed on, without lack or excess, to the next enzyme in the metabolic cascade. Finally, I will discuss how breaking the action-reaction symmetry can allow a system described by two scalar fields to exhibit spontaneous breaking of time translation, time-reversal, space translation, and polar symmetries.

Self-organization of bacterial mixtures interacting via quorum - sensing

Alberto Dinelli¹, Jérémy O' Byrne¹, Agnese Curatolo², Yongfeng Zhao³, Peter Sollich⁴, Julien Tailleur¹

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Understanding the self-organization of motile entities is a key problem in active matter, with applications ranging from pattern formation in biological systems to the engineering of soft active materials. Recently, the regulation of motility in bacteria via quorum sensing interactions (QS), i.e. by the local density of their peers, has shown to be a promising pathway to spatial structuring in these systems.

So far, the literature on the topic has mostly focused on single-component active systems; however, in order to obtain more complex structures like the ones encountered in biology, heterogeneity should be accounted for.

Here, we propose an analytical and numerical study of the self-organization of mixtures of QS run-and-tumble particles. We show the emergence of a rich large-scale phenomenology, including static and dynamic patterns.

First, we derive a microscopic condition for restoring action-reaction at the macroscopic scale, which endows the system with an effective free energy functional. The latter allows us to rationalize the static patterns observed in our simulations and to predict the corresponding phase diagram.

On the contrary, in the presence of non-reciprocal interactions we derive a sufficient condition to observe the emergence of travelling patterns, from steady travelling waves to intermittency and band chaos.

[1] A. Dinelli, J. O'Byrne, A. Curatolo, Y. Zhao, P. Sollich, J. Tailleur, Self-organization of bacterial mixtures in the presence of quorum-sensing interactions (submitted to PRL)

Osmotic stability and thermal fluctuations of giant unilamellar vesicles

Joakim Stenhammar, Xiaoyan Liu, Emma Sparr, Håkan Wennerström
Lund University, Sweden

The bending energy of the lipid membrane is central to all biological processes involving lipid vesicles, such as endocytosis and exocytosis. Since most biological systems sustain significant concentration gradients, osmotic pressure differences are potentially key players in biological membrane remodeling processes. In a recent paper [Liu *et al.*, *J. Phys. Chem. Lett.*, **13**, 498 (2022)], we demonstrate using single-component giant unilamellar vesicles (GUVs) that the bending energy stored in a GUV can sustain significant external osmotic stresses coming from concentration imbalances between the regions interior and exterior to the vesicle. For sufficient osmotic gradients (>0.15 atm) the vesicles globally deform into a prolate shape, and upon osmotic reversal the collapsed vesicles release the bending energy by forming monodisperse “daughter vesicles” through an endocytosis-like process. The observed deformation is in qualitative accordance with the traditional theoretical picture based on a continuum elasticity description of the membrane. However,

the measured osmotic pressure needed for destabilization of the spherical vesicle is about 6 orders of magnitude higher than predicted by theory. In this talk, I will discuss the possible theoretical causes and practical implications of this large discrepancy, and present recent theoretical efforts in describing the effect of thermal vesicle fluctuations on the shape and stability of GUVs.

[1] X. Liu, J. Stenhammar, H. Wennerström, E. Sparr, J. Phys. Chem. Lett., 13, 498-507 (2022)

10:40 to 11:00 Coffee break

Self-assembly of viral capsids and packing of genome

Jure Dobnikar¹, Tine Curk², James D. Farrell¹, Rudolf Podgornik¹

¹Chinese Academy of Sciences, China

²University of Barcelona, Spain

Assembly of viral capsids containing genetic material, is a key process in viral reproduction cycle. The capsid assembly differs qualitatively among viruses: bacteriophages and double stranded DNA viruses assemble their capsids prior to genome packaging, which is then driven by an ATP packaging motor; the single stranded RNA / DNA viruses package their genomes concurrently with the capsid assembly, resulting in a co-assembly of the virus genome and capsid proteins.

To elucidate the mechanism of DNA packing, we have explored the ground states of an elastic filament confined to a sphere with three competing interactions: elasticity, excluded volume, and steric confinement. Replica-exchange MD simulations combined with energy minimization approaches and domain decomposition protocol based on binormal vector correlations showed that the simple coarse-grained model gives rise to a rich complexity. In contrast to a general assumption that viral DNA is packed in an inverse spool configuration, we show that compartmentalization into multiple domains is preferred: at high densities the ground state structure is a complex arrangement of intertwined rings resembling twisted topological links. Multidomain ordering is known from the structure of chromatin, where the complex protein-DNA interactions drive the segregation of DNA. Here, we have shown that it can emerge in a much simpler and smaller system, in the absence of specific structural constraints. The multidomain structure not only minimizes the energy but also strongly affects the kinetics of packing and ejection of DNA from viral capsids.

We have also studied the role of genome topology on the stability of viral capsids in co-assembly process with RNA genome molecules, which feature attractive sites ("*packaging signals*") interacting with capsid proteins. The genome topology (branchiness) has a strong effect on the way the genetic material is distributed inside the shell. It turns out that the optimal capsid size sensitively depends on the branchiness of RNA: straight chains prefer large capsids, while highly branched RNA is optimal for relatively small viruses.

11:00 to 11:20

Hydraulic and electric control of cell spheroids

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¹Matière et Systèmes Complexes, France

²Laboratoire Physico-Chimie Curie, Institut Curie, Paris, France

³Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

On long time scales (several hours or days), cell tissues can rearrange and flow like fluids as a consequence of cell division and cell death. They are unconventional fluids, which can generate forces and react to mechanical cues. Importantly, tissues are also capable to actively pump fluid and create electric current. In this talk, we will discuss how a hydraulic or electrical perturbation, imposed for instance by a drain of micrometric diameter, can be used to perturb tissue growth [1]. We address this issue in a continuum description of a spherical cell assembly that includes the mechanical, electrical and hydraulic properties of the tissue [2,3]. This approach allows us to discuss and quantify the effect of electrohydraulic perturbations on the long-time states of the tissue. We highlight that a moderate external pumping or electric current can drive a proliferating spheroid to decay. We propose that this could have applications in medicine.

[1] C. Duclut, J. Prost, F. Jülicher, PNAS **118**, e2021972118 (2021).

[2] C. Duclut, N. Sarkar, J. Prost, F. Jülicher, PNAS **116**, 19264 (2019).

[3] N. Sarkar, J. Prost, F. Jülicher, New J. Phys. **21**, 043035 (2019).

11:20 to 11:40

The nanocaterpillar's random walk or how to move with jiggly and sticky feet

Sophie Marbach

New York University, United States

Particles with sticky feet - or nanoscale caterpillars - in biological or artificial systems, beat the paradigm of standard diffusion to achieve complex functions. Some cells (like leucocytes) use ligand-receptor contacts (sticky feet) to crawl and roll along vessels. Sticky DNA (another type of sticky feet) is coated on colloids to design programmable interactions and self-assembly. Predicting the dynamics of such sticky motion is challenging since sticky events (attaching/detaching) often occur on very short time scales compared to the overall motion of the particle. Even understanding the equilibrium statistics of these systems (how many feet are attached in average) is largely uncharted. Yet, controlling the dynamics of such particles is critical to achieve these advanced functions -- for example facilitating rolling is critical for long-range alignment of DNA coated-colloids crystals. Here we present advanced theory and experimental results on a model system. We rationalize what parameters control average feet attachment and how they can be compared to other existing systems. We investigate furthermore how various motion modes (rolling, sliding or skipping) may be favored over one another.

[1] Sophie Marbach, Jeana Aojie Zheng, Miranda Holmes-Cerfon-arxiv-to appear in Soft Matter, but also <https://arxiv.org/abs/2111.06468>; <https://arxiv.org/abs/2112.05266>;

11:40 to 12:20

Structure and dynamics of models of (active) responsive colloids

Joachim Dzubiella

University of Freiburg, Germany

Responsive and active particles, as typically found in biology, have received considerable attention recently due to their fascinating (nonequilibrium) physics as well as their high potential in the development of soft functional materials. Here, I discuss coarse-grained models of responsive colloids (RCs) in which the dynamical response of an internal degree of freedom (DoF) or 'property', e.g., the size, of the macromolecule is explicitly resolved and follows overdamped dynamics according to an internal 'parent' energy landscape. I summarize results on how such a dynamical responsiveness influences the collective structure and dynamics of dispersions of RCs, in particular,

how the transition kinetics of internally bistable systems is modified collectively by spatial packing (self-crowding). I further show that rich structure and dynamics emerge if we activate the internal DoF by introducing nonequilibrium fluctuations. Finally, I bridge to a more coarse-grained model of internally active macromolecules in which a discrete, two-state switching of the size and pair potentials of the colloids tunes their diffusive dynamics as well as liquid-liquid micro-phase separation.

4. Posters

Poster 01

A liquid between two and three dimensions

Alvaro Domínguez

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It is well established that, unlike for a three-dimensional fluid, particle interactions prevent the hydrodynamic transport coefficients from being defined for a two-dimensional liquid due to the notorious "long-time tail" feature of the velocity autocorrelation.

In order to address the transition from two up to three spatial dimensions, we study, as a very simple model, the case of a colloidal monolayer at a fluid interface: while the colloidal particles are constrained to a two-dimensional manifold, the exchange of particle momentum, mediated by the ambient fluid in the form of hydrodynamic interactions, takes place in the three-dimensional space.

Starting from the Smoluchowski equation for the system, we show that diffusivity, the only hydrodynamic transport coefficient for this system, exhibits an intermediate behavior between purely two and fully three dimensional colloids: for the monolayer, Fick's law breaks down [1,2] but self-diffusion is finite [3], albeit with a non-analytic dependence on the colloidal packing fraction [A. Domínguez, unpublished]

[1] J. Bleibel, A. Domínguez, F. Günther, J. Harting, M. Oettel, *Soft Matter*, **10**, 2945-2948 (2014)

[2] J. Bleibel, A. Domínguez, M. Oettel, *Phys. Rev. E*, **95**, 032604 (2017)

[3] R. Peláez, F. Usabiaga, S. Panzuela, Q. Xiao, R. Delgado-Buscalioni, A. Donev, *J. Stat. Mech.*, **2018**, 063207 (2018)

Poster 02

A unifying power functional perspective on active and passive liquids

Matthias Schmidt

¹Universität Bayreuth, Germany

The rich and diverse dynamics of liquids ultimately originates from the coupling of their degrees of freedom via internal interactions. To arrive at a tractable approximation of such many-body problems, coarse-graining is often an essential step. Power functional theory [1] provides a unique and microscopically sharp formulation of this concept. The approach is based on an exact one-body variational principle to describe the dynamics of both overdamped and inertial classical and quantum many-body systems. In equilibrium, density functional theory is recovered, and hence spatially inhomogeneous systems are described correctly. The dynamical theory operates on the level of time-dependent one-body correlation functions. Two- and higher-body correlation functions are accessible via the dynamical test particle limit and the nonequilibrium Ornstein-Zernike route. An overview of the structure of this functional approach to many-body dynamics is given, including applications to the van Hove function in liquids, flow in nonequilibrium steady states, and motility-induced phase separation of active Brownian particles.

[1]M. Schmidt, Power functional theory for many-body dynamics, *Rev. Mod. Phys.* (to appear) arxiv: 2111.00432

Poster 03

Active sheets and labyrinths: the phase behaviour of Janus particles in three dimensions

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¹University of Bristol, United Kingdom

²ESPCI Paris, France

³Thin Films Department, Saint-Gobain Research, France

⁴Sapienza University of Rome, Italy

Colloidal systems exhibit phase behaviour equivalent to atoms and molecules yet can be directly imaged in real space with optical microscopy [1]. Recently, it has become possible to produce active colloids [2] which opens the intriguing question as to the interplay between activity and phase behaviour exhibited by equilibrium systems with the same direct interaction potential between the particles [3]. The study of active colloids in experiment has been mostly confined to quasi- two-dimensional systems [4]. In particular Janus particles are self-propelled colloids characterized by the distinct properties of their two hemispheres; in an AC electric field, unbalanced electrophoretic flows produces active Brownian motion with a rich and complex phase behaviour [5]. Here we present an experimental study of the gelation of active Janus particles in three dimensions. Janus particles in an external AC field have a fixed dipole, and if gravity does not dominate over the dipole- dipole interaction, a quasi-two-dimensional active fluid or gas will form long strings in the direction of the field. On reducing the diameter of the particles (to suppress sedimentation), we observed that they do indeed form strings, however, these are but the first point in a completely novel phase space. As the volume fraction is increased, the strings come together into two dimensional sheets, which eventually form a percolating 2d network or 'labyrinth'. Where network formation occurs in this system it is mediated by the activity of the particles themselves, with the gel network decomposing when the field is turned off. Most intriguingly, the structure of this percolating gel is sensitive to the frequency of the applied field. The purpose of this work is to study the mechanism of network formation of Janus particles in three dimensions, and to compare this with simulations and an equivalent passive system.[6][7]. If active systems are to be used in the design of functional materials, an understanding of their phase behaviour is paramount. The study of active gelation has implications in Biology; polar active gels of protein filaments contract in cells to produce movement [8].

[1] A. Ivlev, H. Löwen, G. Morfill, C. Royall, Complex Plasmas and Colloidal Dispersions, (WORLD SCIENTIFIC, 2012)

[2] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, G. Volpe, Rev. Mod. Phys., **88**, 045006 (2016)

[3] M. Marchetti, J. Joanny, S. Ramaswamy, T. Liverpool, J. Prost, M. Rao, R. Simha, Rev. Mod. Phys., **85**, 1143-1189 (2013)

[4] J. Yan, M. Han, J. Zhang, C. Xu, E. Luijten, S. Granick, Nature. Mater., **15**, 1095-1099 (2016)

[5] Nariaki Sakai, C. Patrick Royall, Active Dipolar Colloids in Three Dimensions: Strings, Sheets, Labyrinthine Textures and Crystals, ArXiv

[6] C. Royall, S. Williams, H. Tanaka, J. Chem. Phys., **148**, 044501 (2018)

[7] W. Poon, J. Phys.: Condens. Matter, **14**, R859-R880 (2002)

[8] F. JULICHER, K. KRUSE, J. PROST, J. JOANNY, Physics Reports, **449**, 3-28 (2007)

Poster 04

Assembly and disassembly of passive and active patchy particle architectures

Peter Bolhuis, Hannah Jonas, Peter Schall

¹University of Amsterdam, Netherlands

Synthetic colloidal patchy particles immersed in a binary solvent mixture can self-assemble via critical Casimir interactions into various superstructures, such as chains and networks, which can be explored as model systems to investigate activated viscoelastic architectures, analogous to living matter. To establish a quantitatively accurate potential model that can simulate and predict the experimentally observed equilibrium behavior precisely, we took as an ansatz a general model based on theoretical Casimir potentials and angular switching functions, and optimized several material-specific parameters in the model to match the experimental chain length distribution and persistence length with the predicted ones from Monte Carlo simulations [1]. Using these optimized potentials in large scale simulations, we can predict the phase behavior of mixtures of patchy particles, as well as the conformational behavior of colloidal molecules. In addition, we explain the experimentally observed anomalous monomer fraction using an extended version of Wertheim's thermodynamic perturbation theory [2]. Finally, we take the system out of equilibrium, by including self-propelled particles, causing chains in the network to undergo breakage and rearrangement. Employing Brownian dynamics, we study the response of the kinetics of breakage as a function of activity, giving insight into the non-equilibrium physics of activated viscoelastic architectures.

[1]H.J. Jonas, S.G. Stuij, P. Schall, and P.G. Bolhuis, J.Chem.Phys. 2021,155,034902

[2]H.J. Jonas, S.G. Stuij, P. Schall, and P.G. Bolhuis, in preparation

Poster 06

Capillary wave theory in active systems: a field theoretical analysis

Cesare Nardini

¹CEA, France

In passive fluid-fluid phase separation, a single interfacial tension sets both the capillary fluctuations of the interface and the rate of Ostwald ripening. We show that these phenomena are governed by two different tensions in active systems, and compute the capillary tension which sets the relaxation rate of interfacial fluctuations in accordance with capillary wave theory and the spectra of interfacial fluctuations which we characterise both at linear (weak fluctuations) and non-linear level (strong fluctuations). Furthermore, we discover that strong enough activity can cause negative capillary wave interfacial tension. In this regime, depending on the global composition, the system self-organizes, either into a microphase-separated state in which coalescence is highly inhibited, or into an “active foam” state. Our results are obtained for Active Model B+, a minimal continuum model which, although generic, admits significant analytical progress.

Poster 07

Cavitation of fluids under tension in nanopores

Joël Puibasset

¹CNRS, France

The extreme confinement of fluids in nanopores strongly affects their properties, which has measurable consequences even at the micrometer scale. One can cite the effect of surface chemistry or corrugation, local curvature, pore morphology, or any other nanometer-scale property of the surface. Molecular simulation is a powerful route to address such issues since it takes into account the relevant fluid/fluid and fluid/substrate interactions at the atomic scale.

An interesting issue is the out-of-equilibrium pore emptying, in particular in the case of the so-called inkbottle pores that are connected to the outside only through narrow channels. Focusing on the molecular simulation of fluids confined in chemically disordered pores, we will show how the heterogeneities induce the appearance of metastable states, and how these states can be used to study cavitation in inkbottle pores. The simulations are compared to the classical nucleation theory, through the direct evaluation of the nucleation rate and the barrier height. The results are relevant to experiments showing that in such pores desorption proceeds via liquid fracture (cavitation).

Poster 08

Characterization of the auto-assembly of electronic surfactants at the liquid–gas interface

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The environmental costs associated with the semiconductor make its sustainability a challenge. In an effort to spearhead new alternatives, the PROGENY project is trying to create proto-electronic devices using soap bubbles.

In order to achieve this vision, a fundamental step is to design a new kind of surfactants, that can elicit long range electronic conduction within the surfactant monolayer of a bubble Figure 1.

We use Langmuir trough and optical techniques such as Ellipsometry or Second Harmonic Generation, to understand the self-organization of new, purpose designed, surfactants at the air–water interface, as a function of surfactant concentration. These characterizations and associated modeling of the surfactants allow us to investigate the presence of π -stacking, which is a path to conduction [1], to improve foamability of the surfactants, and to understand their behaviour.

In this poster, I will present how the combination of these techniques allows us to give insight into these properties.

[1] S. Schneebeli, M. Kamenetska, Z. Cheng, R. Skouta, R. Friesner, L. Venkataraman, R. Breslow, J. Am. Chem. Soc., **133**, 2136-2139 (2011)

Poster 09

A competitive advantage through fast dead matter elimination in cellular soft matter

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¹MPI-NAT, MPI-DS, Göttingen, Germany

²Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Göttingen, 37077, Germany

Competition of different cell types for limited space is relevant in biological processes such as tissue morphogenesis and tumor growth. Predicting the outcome for non-adversarial competition of such growing active matter is non-trivial, as it depends on how processes like growth, proliferation and the degradation of cellular matter are regulated in confinement; regulation that happens even in the absence of competition to achieve homeostasis. We show that passive by-products of the processes maintaining homeostasis can significantly alter fitness, enabling cell types with lower homeostatic pressure to out-compete those with higher homeostatic pressure. Using both a theoretical toy model

and an agent-based computational model that include finite-time mechanical persistence of dead cells, we reveal that interfaces play a critical role in the competition: There, growing matter with a higher proportion of active cells can better exploit local growth opportunities that continuously arise as the active processes keep the system out of mechanical equilibrium. Our results show that optimizing the proportion of growing (active) cells can be as important to survival as sensitivity to mechanical cues.

[1] Y. Pollack, P. Bittihn, R. Golestanian, A competitive advantage through fast dead matter elimination in confined cellular aggregates, 2021

Poster 10

Clustering versus fluctuations in monohydroxy alcohols

Martina Požar

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It is well known that monohydroxy alcohols, such as methanol or octanol, tend to form chain-like clusters, principally due to the charge ordering induced by the OH hydroxyl groups, the oxygen being negatively charged, and the hydrogen positively charged. This local order can be detected by radiation scattering [1,2,3]. What is less known is how the alkyl tails influence this local ordering. This topic can be studied by increasing the alkyl tails of the monohydroxy alcohols, from methanol all the way to undecanol, and the variation of the pre-peak monitored through computer simulations. By calculating the various atom-atom correlations and rebuilding the X-ray scattering spectra, we demonstrate that the flexibility of the alkyl tails with increasing sizes play a predominant role in determining the variation of the scattering pre-peak [4]. The influence of branching in the alkyl tail is equally studied for the case of octanol [5]. It is shown that the flexibility produces a transition in the pattern of chain ordering, which is related to the fluctuation of the methyl/methylene “field” surrounding the chained hydroxyl groups, and which occurs around 1-pentanol. This is an illustration of the hardness/softness change of meta-particles which are formed by the clustered entities within pure monomeric liquids.

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[5] J. Bolle, S. Bierwirth, M. Požar, A. Perera, M. Paulus, P. Münzner, C. Albers, S. Dogan, M. Elbers, R. Sakrowski, G. Surmeier, R. Böhmer, M. Tolan, C. Sternemann, Phys. Chem. Chem. Phys., **23**, 24211-24221 (2021)

Poster 11

Coarse-graining many-body interactions of ligand-stabilised nanoparticles using machine learning

Giuliana Giunta, Gerardo Campos-Villalobos, Marjolein Dijkstra

¹Utrecht University, Netherlands

Colloidal nanoparticles can self-assemble into a variety of two-dimensional and three-dimensional superstructures with unique optical, structural and electronic properties. [1] These nanostructured materials have a large surface-to-volume ratio, which makes them useful in different fields, ranging from opto-electronic, plasmonic, and photonic applications, to catalysis and batteries. To prevent aggregation in the solvent, nanoparticles are stabilised by a capping layer of organic ligands. Therefore, the type of ligand, the solvent-ligand interactions and the temperature can influence the

effective interactions between the nanoparticles and ultimately their self-assembly. To understand the kinetic, equilibrium properties and the influence of temperature and solvent quality on the effective interactions of the nanoparticles, we perform molecular dynamics simulations using simple and computationally efficient coarse-grained (CG) models of gold nanoparticles coated with alkyl chains. For specific size ratios between the dimension of the ligands and the nanocrystal core, at small particle separation, the effective force between pairs of particles is largely affected by the presence of neighbouring particles. Thus, many-body effects are relevant and should not be neglected when building up CG models for the nanoparticles. In our research, we employ a machine-learning approach to construct many-body interaction potentials for ligand-stabilised nanocrystals that can be used in computer simulations to investigate their phase and self-assembly behaviour.

[1] P. Schapotschnikow, R. Pool, T. Vlucht, *Nano Lett.*, **8**, 2930-2934 (2008)

Poster 12

Collisions enhance self-diffusion in odd diffusive systems

Abhinav Sharma, Erik Kalz, Hidde Vuijk, Iman Abdoli, Jens Sommer, Hartmut Löwen

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It is generally believed that collisions of particles reduce the self-diffusion coefficient. Here we show that in odd-diffusive systems, which are characterized by diffusion tensors with antisymmetric elements, collisions surprisingly can enhance the self-diffusion. In these systems, due to an inherent curving effect, the motion of particles is facilitated, instead of hindered by collisions leading to a mutual rolling effect. Using a geometric model, we analytically predict the enhancement of the self-diffusion coefficient with increasing density. This counterintuitive behaviour is demonstrated in the archetypal odd-diffusive system of Brownian particles under a Lorentz force. The physical interpretation is quantitatively supported by the force-autocorrelation function, which turns negative with increasing odd-diffusivity. We validate our findings by many body Brownian dynamics simulations in dilute systems.

Poster 13

Colloidal crystallisation under the influence of an external electric field

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Colloidal suspensions exhibit rich phase behaviour under the influence of external electric fields. They have been shown to form structures such as string fluids, body centred cubic (bcc), face centred cubic (fcc), body centred orthorhombic (bco), space filling tetragonal (sft) and body centered tetragonal (bct) [1]. The colloidal suspension used in this study can be modelled by Yukawa interaction under zero field. In the presence of an external electric field, each colloidal particle gains a net dipole moment due to the charge polarisation and results in a net anisotropic, dipolar interaction.

Although the equilibrium phase behaviour of this system has been studied extensively by experiments and simulations [1,2], there has yet to be a detailed quantitative analysis of its crystallisation behaviour. In this work, we are employing particle-resolved studies in 3D via confocal

microscopy to record the nucleation and growth of the colloidal crystals under the influence of the external AC electric field. By applying bond order parameters analysis and the Topological Cluster Classification (TCC) on the tracked particles [3], we are able to quantify and monitor the clusters formation and crystallinity of the colloidal suspension undergoing crystallisation, hopefully drawing a link between the symmetry of these clusters and the final rich crystal structures and morphologies exhibited by such dipolar system.

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Poster 14

Combining force inference and holographic microscopy to measure colloidal interactions

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There are two types of methods to extract the forces acting on colloids: equilibrium- distribution and drift-diffusion methods [1,2,3]. While the former can only be used when the system is in thermodynamic equilibrium, drift-diffusion methods relying on displacement measurements do not require this condition. Alas, because of the solvent agitation deterministic displacements caused by the forces are tangled with Brownian motion and when this thermal noise is heterogeneous, particles are subject to a noise-induced spurious force that adds another layer of complexity [4,5]. Recently, a novel method based on information and communication theory was introduced to infer force-fields and diffusion from high dimensional stochastic trajectories [6] Within this approach, we develop a framework for the analysis of trajectories of individual colloids: we first validate our approach with molecular dynamics simulations and we then successfully apply it to three-dimensional trajectories of individual colloids measured using a modified version of 3D-phase contrast holographic microscopy [7]. Within this framework we are able to infer the one-body and two-body interactions as well as the diffusion and spurious force in different solvents. Our method also allows to investigate the measurement error to optimize the acquisition protocol.

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[3] I. Jenkins, J. Crocker, T. Sinno, *Soft Matter*, **11**, 6948-6956 (2015)

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[5] G. Volpe, J. Wehr, *Rep. Prog. Phys.*, **79**, 053901 (2016)

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[7] F. Cheong, C. Wong, Y. Gao, M. Nai, Y. Cui, S. Park, L. Kenney, C. Lim, *Biophysical Journal*, **108**, 1248-1256 (2015)

Poster 15

Consistent local stress theory of discrete particle systems

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²MPIKG, Germany

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In this work we are interested in the definition of stress in molecular dynamics systems. Current theory recognizes two objects as the stress tensor: i) the Cauchy stress tensor from continuum elasticity and ii) the local stress tensor derived as the solution to the local-stress equation based on the Irving-Kirkwood-Noll (IKN) procedure. The Cauchy stress tensor is a unique tensor that describes the forces acting on a surface element of a body. In contrast, the local stress tensor is not unique, because the defining differential equation lacks boundary conditions to select a unique solution. Many have attempted to impose additional requirements to single out a unique local stress tensor; however, no consensus has been reached.

We present a new approach to derive mechanical work for a discrete particle system under constant-entropy deformations. This results in a mechanical work equation (MWE) which is unique, non-local and shows that all IKN stress tensors are equally relevant physically as long as a corrected expression for the mechanical work is used. Under specific circumstances, the new MWE is equal to the conventional equations. One is when the surface tension is calculated, explaining why the IKN procedure there yields correct results. However, the new MWE's non-locality prevents the stress tensor from being interpreted as in elasticity theory, i.e., as a Cauchy stress tensor. In conclusion, the key insight is that in discrete particle systems there exists no local stress, i.e., an object that has all properties of the Cauchy stress tensor; however, because of the mechanical work equation, such a tensor is also not necessary.

Poster 16

Cybotactic order in molecular liquids

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Cybotactic order concerns the appearance of strongly correlated small domains in equilibrium molecular liquids. Various forms of cybotactic order exist. Hydrogen bonded clusters in aqueous mixtures, or in neat alcohols, smectic rafts in nematic liquid crystals, solvation layers in solutions, or micelles in micro-emulsions, can be considered as different forms of the cybotactic order. Because of the dual fluctuation/clustering ambiguous nature of this form of local order, cybotacticity is often at the verge of non-equilibrium or metastability, with inevitable kinetic issues associated with it. We propose a formalism based on the statistical theory of liquids which describes for this form of local order, in particular in the pair correlation functions. It accounts for the experimental signatures of the cybotactic order, as seen from radiation scattering in molecular liquids.

Poster 17

Defects and nucleation in charged colloids

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Suspensions of charged colloids are among the most fundamental systems in colloidal science. Due to their straightforward realization in the lab and impressive agreement with computational and theoretical studies, these systems have been instrumental in enhancing our understanding of both atomic and colloidal crystals. Nonetheless, despite the century-long investigation into charged colloids, their behavior can still surprise us.

In this talk I will discuss two well-kept secrets of charged colloids related to crystal nucleation and point defects. With respect to nucleation, I will show that even highly screened charge interactions can clearly change the nucleation free-energy barriers of (almost) hard-spheres, bringing into question to what extent well-screened charged particles can ever be considered to behave like hard spheres in the context of crystal nucleation. Additionally, I will discuss how defects manifest in both face-centered cubic (FCC) and body-centered cubic (BCC) crystals of charged colloids. I will show that point defects are predicted to occur in surprisingly high concentrations in the BCC crystal, and that the interstitials in the BCC crystal form exotic, one-dimensional, long-ranged deformations called crowdions [1].

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Poster 18

Dense granular flows on inclined planes

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We theoretically address the steady state of thick and dense granular flows atop inclined planes. From Discrete Element Method numerical simulations, we investigate how the inclination angle influences the flow properties. The results are broadly compared to experimental and numerical data from the literature, as well as to the $\mu(I)$ -rheology empirical relations. In particular, the low-inertial-number regime is rationalized through a novel theoretical approach combining two main ingredients: diffusion properties and cooperative effects. This nonlocal feature appears as an essential ingredient in order to explain the data and explain the commonly used empirical laws.

Poster 19

Depletion-induced crystallization of triblock biaxial colloids

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The presence of depletants in a colloidal solution typically generates short-range attractive interactions. These can be exploited to assemble colloids into different types of structures with peculiar properties and applicative interests for example in the field of photonics. A better control and a more precise directionality of the assembly can be obtained by acting on the structure of the colloids, as it has been demonstrated through the so-called lock-and-key mechanism or by acting on the surface roughness of the particles [1]. In addition, the combined use of materials that respond differently to the presence of depletants due to surface charge and particle-depletant interaction effects can be exploited for this purpose [2].

Here, we study numerically a system consisting of biaxial colloids whose extremities and central parts mimic the use of different types of materials. In this way, we determine the optimal conditions for the formation of crystalline patterns in quasi two-dimensions, which vary depending on the ratio between the two axes of the particles. By tuning appropriately depletant size and surface charge of the colloids, the crystalline structures are favored over the formation of gel percolating networks

where random arrangements prevail. In addition to the formation of structures on a substrate, which comprises brick-walls and herringbone patterns, we study the assembly of such biaxial colloids in bulk. In particular, we exploit the previously assembled crystalline layers as templates for the formation of three-dimensional structures, obtained by depositing colloids by gravity. This study demonstrates the potential of combining different materials together with depletion interactions for the self-assembly of anisotropic colloids and provides guidance for their experimental attainment at the fundamental and applied levels.

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Poster 20

Design smart polymeric materials for controlled, selective and reversible adsorption at the nanoscale

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Designing nanomaterials for selective and tunable adsorption/release is a topic of extremely wide interest, with a manifold of possible applications, spanning from biomedical ones, with the realisation of functionalised systems for drug delivery [1], up to more applied materials for selective removal of contaminants in water [2]. The creation of a pipeline leading to the design, and consequent realisation, of the optimal material, requires a multidisciplinary approach, as a multitude of details, from the atomic up to the meso scale, have to be considered. With this talk, we will show a generalised path that, starting from atomistic simulations - tailored on experimental synthesis - passes through a multiscale theoretical and computational process, and finally reaches its final experimental goal, with the realisation of functionalised nanoparticles with fully controllable and tunable properties. Through a hybrid theoretical and experimental approach, we will show how to choose and tune atomistic details in general classes of polymers to assess the optimal sub-category of polymeric adsorbers. A multiscale strategy will then be implemented to assess how to exploit the selected optimal polymeric classes by assembling them in polymeric macromolecules, and specifically how to unveil the role played by the geometry of the macromolecules in both adsorption and selectivity [3]. We will then show that it is possible to define universal classes of adsorbers just retaining a few microscopic details [4]. Finally, we will present an experimental realisation of a designed nanomolecular adsorber [5,6].

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Poster 21

Diffusio-osmotic transport of hydrophobic solutes and slippage opacity of two-dimensional materials

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Understanding the nature of the interactions of liquids on solid surfaces is key to achieve molecular control over solute transport at aqueous interfaces in nanofluidics and, therefore, can lead to important advances for water purification. We propose a framework to compute the diffusio-osmotic transport of hydrophobic particles at aqueous interfaces from equilibrium molecular dynamics simulations by combining the Stokes equation of hydrodynamics with the theory of the hydrophobic effect [1]. We describe the free energy of hydration of small solutes from the probability of formation of a cavity at the interface. Within this model, the fluid velocity is obtained according to Stokes equation[2], which is modified to account for the liquid/solid friction, resulting in water slippage. We apply this framework to investigate the diffusio-osmotic transport of small hydrophobic solutes at several aqueous interfaces of interest in nanofluidics by means of extensive ab initio molecular dynamics simulations. In particular, we focus on the aqueous single and bilayer graphene, hBN and MoS₂ interfaces, as well as their bilayer heterostructures. We show that, despite the adsorption free energy on different interfaces remains the same, the diffusio-osmotic coefficient of the hydrophobic particle can change dramatically. For instance, it is around an order of magnitude larger when water is in contact with graphene with respect to when it is in contact with MoS₂. Therefore, we conclude that the diffusio-osmotic coefficient is heavily controlled by slippage, which can be very different and is influenced only by the layer being in direct contact with water. Further, we investigate the structure of water for every system and show how it impacts the free energies of solvation of a hydrophobic solute. Our work is a first step into the design from first principles of materials which promote fast water slippage for applications in coatings and water purification nanofluidic membranes.

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Poster 22

Drying-induced bending of hydrogel disks

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Hydrogel actuators are typically made of a bilayer gel that can promote water diffusion in one of the layers, subsequently inducing bending. Here, we show that a similar bending behavior can be achieved by simply drying a hydrogel disk on a substrate. By varying the gel's aspect ratio and the substrate surface energy we are able to either observe (1) a deposit stuck to the substrate, (2) the bending of the hydrogel disk, or (3) planar drying until buckling of the disk occurs. We explain our results using a simple energy balance between the drying-induced elastic energy stored in the gel and the adhesion energy of the substrate. We then investigate in more details the bending phenomenon using numerical simulations allowing us to capture the drying dynamics of hydrogel disks. Together, our results provide both fundamental and application insights on, e.g., the drying-induced buckling of thin disks, an active field of research in the colloidal suspension community; and the design of new actuators, sensors, or even origami using differential drying.

Poster 23

Dynamics and microrheology of diluted suspensions of cubic particles under an external electric field

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Colloidal suspensions (or simply sols) are biphasic systems composed of a solid phase that is homogeneously dispersed in a liquid medium, in domains of size within a few nanometres to a few micrometres. Sols are especially relevant in formulation science as they form the basis for a number of products of daily usage, including detergents, paints, coatings and foods.

When an external electric field is applied to a sol, and the permittivity of the two phases is different, the colloidal particles composing the dispersed phase are polarised. The induced dipoles generated by external fields enhance particles attraction, which cause microscopic reorganization of the dispersed phase and the formation of oriented string-like clusters or chains. These chains have been observed in suspensions of both spherical [1] and anisotropic dielectric particles [2]. Such a directed self-assembly has relevant consequences in the rheological properties of the entire suspension. Under some specific conditions, where volume fraction, dielectric properties and field intensity play a crucial role, the viscosity of the colloidal suspension can change drastically [3]. Electrorheological (ER) fluids have technological applications in dampers, clutches, brakes, electronics.

In this work, we perform Dynamic Monte Carlo simulations of an ER fluid made of polarisable cubic particles and investigate the kinetics of formation of chain-like clusters [4]. We analyse the response time of the fluid transitioning from an isotropic state to an oriented string-like state. Additionally, we investigate the main structural properties of the chains that are formed and how they influence the viscoelastic response of the system. More specifically, we apply passive microrheology [5] to compute the viscous and elastic moduli along the direction of the field and perpendicularly to it. Our results clarify the role of chains in determining a change in viscosity and open up a path to evaluate the viscoelastic response of ER fluids by applying efficient simulation methods.

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Poster 24

Dynamics of fluids in random potential energy landscapes: mode-coupling theory and beyond

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The first applications of the scheme that led to the mode-coupling theory of the liquid-glass transition (MCT) dealt with noninteracting fluids in random environments. At the time, a number of strengths and weaknesses of the theory were already apparent. Yet, until recently, these conceptually simpler problems received surprisingly little attention in the various attempts to rederive, improve or extend the MCT within well-defined and controlled approximation schemes. Therefore, as a step in that direction, we developed a field-theoretic perturbation method preserving the fluctuation-dissipation

relation for the dynamics of a noninteracting colloidal gas plunged in a quenched Gaussian random field. The first-order bare theory reproduces the MCT equations for the problem at hand, albeit with a memory integral written in terms of the correlation function of the pure system. It is found to summarize in a simple way many previous results on the long-time tails in fluids in disorder, including those appearing in the density correlation function. A renormalized self-consistent theory was also developed from the bare theory. It shows some structural similarity with the MCT, as a self-closed dynamical equation for the density correlation function is obtained as well. However, its predictions noticeably improve upon those of the MCT. Indeed, it similarly predicts an ergodicity-breaking transition for the density fluctuations, but, at variance with the MCT, a normal diffusive behavior always holds at long time, in agreement with known rigorous results.

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Poster 25

Effect of temperature on slip and friction of liquids at the solid-liquid interface

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A basic assumption of fluid mechanics is the no-slip boundary condition. Nevertheless, in some cases, the fluid slips at the surface and the slippage can be characterized by a slip length b which is the distance in the solid where the velocity profile extrapolates to zero. The slippage is the result of the balance between two different quantities: the bulk viscosity (η) and the friction coefficient between the liquid and the wall (k) which relates the stress τ transmitted to the solid by the liquid to the slip velocity $\tau = kV$. More precisely, Navier [1] has shown that slip length, viscosity and friction can be related by:

$$b = \eta / k$$

In many cases, the friction dominates so that $b \rightarrow 0$ and the no-slip boundary condition is relevant. However, for highly viscous flows or for very small-scale systems, slip cannot be neglected anymore. In this case, how much the liquid slips depends on the molecular interactions of both the liquid and the wall, but the mechanisms underlying these dependencies remain unclear. In particular, the effect of temperature on slippage is still unknown: numerical simulations report non-monotonic slip lengths with respect to temperature [2,3], while experimental measurements have noticed slip lengths either constant or decreasing with temperature [4,5].

We conduct molecular dynamics simulations of a model fluid (Kob-Andersen bi-disperse Lennard-Jones fluid) undergoing a shear flow between two smooth walls. We measure both the viscosity $\eta(T)$ and the friction coefficient $k(T)$ in order to obtain the slip length as a function of temperature $b(T)$. We manage to tune the monotony of $b(T)$ by controlling the interaction energies between the liquid and the solid. This gives a new common framework in which the results of the existing literature could be rationalized.

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Poster 26

Effects of scalar activity on phase transitions of liquid mixtures

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We study two-dimensional binary mixtures consisting of active and passive colloids, by performing molecular dynamics simulations, using two different thermostats. The first part of the talk will discuss the effects of the activity on the liquid-solid phase transition, and on elastic properties of the solid [1]. The second part is focused on properties of phase-separated such systems.

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Poster 27

Entropic differences between lattices formed by hard ellipses

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Hard ellipses in a two-dimensional setup and at high packing fractions show an intricate variety of possible lattice conformations [1]. These structures all emerge from a hexagonal arrangement of disks via suitable deformations along a chosen axis. We characterize the resulting lattice types by two parameters, namely ω and τ , which specify orientational and positional order of the particles.

We show that for ellipses with aspect ratio $\kappa = 2$ only two relevant lattice types survive within the plethora of possible ordered configurations. Our simulation-based investigations rely on lattice-switch Monte Carlo moves, so that the underlying parameter space of lattice configurations is directly probed. By investigating the entropic landscape we find that ordered lattice types characterized either by $\omega = 0^\circ$ - named the diagonal lattice state - or $\omega = 30^\circ$ - named the parallel lattice state - are the most stable ones.

In an effort to find the true ground state, i.e. the global entropy-maximum, the exact entropic difference between the parallel and the diagonal state is computed. We achieve this with the help of complementary computational methods, such as a Potential Mean Force Method in combination with the Reweighting Histogram Technique [2] as well as the Einstein Crystal Method [3]. Our results show that the diagonal lattice-state is entropically favoured over the parallel one for systems sizes of up to sizes of approximately 400 particles. We find evidence that this entropic difference persists also in the thermodynamic limit.

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Poster 28

Failure behavior in catch bond networks

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Most of the bonds observed in polymer systems often exhibit slip behavior, i.e., they weaken under the action of mechanical load. In this way, the dissociation rate grows with increasing forces. However, Nature shows us through cell adhesion or cellular mechanosensing the existence of a surprising behavior: Some proteins establish links that stiffen at moderate tensions, thus prolonging their lifetime [1,2]. These links, named catch bonds, represent a novel mechanism to control the failure behavior in biopolymer systems still unexplored.

In this contribution, we address this problem using athermal simulations of 2D transient networks under uniaxial deformation, where bonds can be immobile or mobile [3]. Thus, whereas immobile bonds always form in the same network location, mobile ones can establish new links in different places [4]. Then, we find that the combination of mobile and catch bonds translates into a remarkable delay in network failure. Then, to decipher how the fracture is developed, we focus on the crack nucleation and propagation under deformation, finding that the presence of slip bonds induces a brittle behavior, characterized by a prevalent crack that expands up to percolate. On the other hand, catch bonds cause a ductile behavior clearly marked by creating many cracks that finally merge, leading to a fracture.

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Poster 29

Frequency-dependent electrical impedance of nanocapacitors from molecular dynamics simulations

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Understanding the microscopic behaviour of electrode-electrolyte interfaces is crucial for several applications, including energy storage and electrocatalysis [1]. In this context, the polarization of the electrode can reveal precious insights related to the thermodynamic, static and dynamical properties of the electrolyte, and molecular simulations have become an essential tool of investigation. For example, using classical molecular dynamics, we recently showed the importance of charges induced on electrode atoms and how they are related to the static properties of electrode-electrolyte interfaces [2].

In previous work, we showed how to extract the capacitance and the evolution of the structure of the interface as a function of voltage from the fluctuations of the total charge of the electrode [3,4]. Here, we extend this approach to compute the complex impedance/admittance of the system as a function of frequency from the dynamics of the electrode charge fluctuations. The impedance/admittance can be measured in electrochemical experiments and molecular simulations may provide a link between these quantities and the interfacial dynamics. We illustrate this method on molecular dynamics simulations of nanocapacitors consisting of pure water or a water-NaCl solution between gold electrodes. We show in particular how the electrical behaviour is related to the electrolyte dynamics and how it depends on the physical properties of the system, such as the distance between the electrodes or the presence of ions.

This work is part of the ERC project SENSES (grant No. 863473). Project website: <https://benrotenberg.github.io/erc-senses/>

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Poster 30

From a microscopic inertial active matter model to the Schrödinger equation

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Field theories for the one-body density of an active fluid, such as the paradigmatic active model B+, are simple yet very powerful tools for describing phenomena such as motility-induced phase separation. No comparable theory has been derived yet for the underdamped case. In this work, we introduce active model I+, an extension of active model B+ to particles with inertia. The governing equations of active model I+ are systematically derived from the microscopic Langevin equations. We show that, for underdamped active particles, thermodynamic and mechanical definitions of the velocity field no longer coincide and that the density-dependent swimming speed plays the role of an effective viscosity. Moreover, active model I+ contains the Schrödinger equation in Madelung form as a limiting case, allowing to find analogs of the quantum-mechanical tunnel effect and of fuzzy dark matter in the active fluid. We investigate the active tunnel effect analytically and via numerical continuation.

Poster 31

Guiding the assembly of colloidal diamonds

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The assembly of cubic colloidal diamonds has drawn special attention in previous years as their possible use as photonic crystals. The process of their assembly is still challenging since the regions where stable cubic diamonds are elusive. To enhance its self-assembly the usage of tetrahedral directional interactions¹ and anisotropic particles with tetrahedral shape² has been widely explored. Recently, these two main approaches were combined and studied in experiments² where a tetrahedral-like particle was devised with the addition of DNA-coated patches. The main interactions leading the assembly were the strong directional interaction due to the DNA patches and depletion found in the experiments.

Here, we explore in detail the role of depletion on the formation of colloidal diamonds in a similar model with the use of molecular simulations. We show that the region of parameters where stable colloidal diamonds is found is quite narrow, being an interplay between the strength of the depletion interaction and its range. Moreover, we found that outside this stable region the system is arrested due to the short attractive interactions, forming a percolating gel-like network with an internal crystalline structure. Interestingly, we demonstrate that the cubic colloidal diamond can be still assembled without the strong directional interaction due to DNA, being the self-assembly a process mainly mediated by the depletion and the anisotropy of the particles. With these results we provide a clearer route to assemble cubic colloidal diamonds.

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Poster 32

Hydrophobic hydration at the molecular scale: the key role of hydrogen-bond distortion

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Understanding the structural and thermodynamic properties of water around hydrophobic solutes is key for such important processes as protein folding or the design of advanced materials. In the textbook picture [1,2], small hydrophobes can be accommodated by the water hydrogen-bond (HB) network, only leading to a restriction of water molecule configurations (with a solvation free-energy dominated by an entropic contribution). As the solute grows in size, a crossover would be observed to a regime similar to a liquid/vapor interface, with the formation of dangling hydrogen-bonds and a solvation free-energy dominated by the associated enthalpic cost in the form of a surface-tension. However, a detailed analysis of the associated changes in the water HB network around realistic solutes is still missing.

Using molecular dynamics simulations and simulated vibrational spectra on a variety of solutes of increasing size, including model repulsive cavities, fullerenes, and amphiphilic solutes, we show that the famous thermodynamic crossover is indeed observed for repulsive cavities, but not for realistic hydrophobic solutes, where it is masked by attractive interactions. However, the structural changes occurring in the HB network are very similar around model cavities and realistic solutes, with a continuous HB network rearrangement when the solute/cavity grows in size, without sharp transition. We show that this HB network progressive rearrangement is what was observed in recent Raman experiments. [3] We find that the previously under-appreciated distortion of the intact HB network plays a key role in the solvation thermodynamics, equally as important as the formation of dangling HBs. This distortion is reflected in the hydration thermodynamics and dynamics, and also explains the temperature-dependence of hydrophobic hydration. With this new picture, we show that the surface-tension of water is only partly due to broken HB at the interface, and that distorted HBs account for a significant fraction of the free-energy cost associated with an interface formation.

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Poster 33

Kinetic theory of a confined quasi-one-dimensional gas of hard disks

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A dilute gas of hard disks confined between two straight parallel lines is considered. The distance between the two boundaries is in between one and two particle diameters, so that the system is quasi-one-dimensional. A Boltzmann-like kinetic equation, that takes into account the limitation in

the possible scattering angles, is derived. It is shown that the equation verifies an H theorem implying a monotonic approach to equilibrium. The implications of this result are discussed, and the equilibrium properties are derived. Closed equations describing how the kinetic energy is transferred between the degrees of freedom parallel and perpendicular to the boundaries are derived for states that are homogeneous along the direction of the boundaries. The theoretical predictions agree with results obtained by means of molecular dynamics simulations.

Poster 34

Kinetic theory of fluids under strong confinement

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A kinetic equation for a system of elastic hard spheres or disks confined by a hard wall of arbitrary shape is derived. It is a generalization of the modified Enskog equation in which the effects of the confinement are taken into account and it is supposed to be valid up to moderate densities and to describe the liquid state. A Lyapunov functional, $H[f]$, is identified. For any solution of the kinetic equation, H decays monotonically in time until the system reaches the inhomogeneous equilibrium distribution, that is a Maxwellian distribution with the density field consistent with equilibrium statistical mechanics. From the equation, balance equations for the hydrodynamic fields are derived, identifying the collisional transfer contributions to the pressure tensor and heat flux. This let us to formulate a generalization of the wall theorem to arbitrary non-equilibrium states [1].

The theory is applied to the extreme case in which the system is confined between two hard walls separated a distance smaller than twice the diameter of the particles. In this case, the particles can not jump over each other and the system can be considered to be quasi-two-dimensional [2].

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Poster 35

Local entropy/energy fluctuations in molecular liquids: the role of the site-site bridge function

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The description of liquids through pair correlations requires to include higher order correlations through the so-called bridge function [1, 2]. This contribution can be considered as accounting for fluctuations as seen from pair level description. Neglecting these contributions reduces the pair level description to mean field type. For simple liquids and their mixtures, atomic or molecular, it is found that these bridge contributions are rather small [3, 4]. For complex liquids, however, the comparison between exact pair correlations (as obtained from simulations) and approximate ones where the bridge is neglected, is often catastrophic [5, 6, 7, 8]. This is particularly true for mixtures, for which it is often impossible to obtain numerical solutions [9, 10, 11].

The bridge function can be calculated from simulations, both for the molecular [12] and atom-atom versions [8] of the integral equation theory (IET), thus making both approaches exact.

In order to better interpret the meaning of the bridge function, we consider that the fluctuations depend on local energy and entropy. This separation allows to intuitively understand the importance of the bridge function in the atom-atom IET: since molecules are represented in atomic details, the energy contribution of the corresponding fluctuations are directly provided into the theory as intra-molecular correlations, without the compensation of the entropy contributions. This does not hold for the molecular theory, where the intra-molecular correlations are not taken into account, leading to a compensation which explains why it has qualitatively better predictions than the atom-atom version. In other words, the need for the bridge function is more important in the atom-atom version of IET.

We test and illustrate this hypothesis in the case of model molecular systems, by tuning the local ordering as to enhance or restrict the corresponding local fluctuations through clustering.

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Poster 36

Long-term memory and synapse-like plasticity in 2d nanochannels

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Fine-tuned ion transport across nanoscale pores is key to many biological processes such as information processing in the brain. Recent experimental advances have enabled the confinement of water down to a single molecular layer between two layers of graphene [1], where electrolytes have been newly predicted to develop millisecond-long memory [2]. In this talk, I will present the first experimental exploration of such phenomena. Our experiments have unveiled hour-long memory, defying previous explanations, with two distinct mechanisms allowing to store information into the pore's conductance. I will also show how this can be fully rationalized using analytical theory describing the system's surface properties. Notably, arbitrarily large timescales can emerge from coupling ion transport to interfacial processes, where the surface charge plays a key role. Fine understanding of the underlying physics has moreover allowed us to design basic experimental implementations of learning algorithms, such as Hebb's rule. This proof-of-concept paves the way for the development of 'iontronics' devices reproducing the functioning of biological systems.

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Poster 37

Machine-learning correlations between structure and dynamics in supercooled liquids and glasses

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One of the most fundamental problems in the field of glass physics is understanding the connection between amorphous, microscopic structure and structural relaxation. While for crystals it is well known that relaxation is induced by well-defined 'defects' in the ordered structure, finding an analogous definition for 'amorphous defects' in glasses remains to be a great challenge. Many physically-motivated structural descriptors have been suggested to predict dynamical properties from structure with good success but it could be shown in recent years that machine-learned descriptors have the potential to be far superior [1,2]. In my talk, I will present a general framework to machine-learn correlations between structure and dynamics in supercooled liquids. I will show that the learned model has significantly higher accuracy than all other techniques that have so far been suggested in the literature and transfer well to lower temperatures. Finally, I will explain how this framework therefore opens up the possibility to understand glassy dynamics at unprecedented low temperatures.

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Poster 38

Machine-learning effective many-body potentials for colloidal systems

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In the past few years, we have witnessed enormous advances in the development of data-driven potentials for simulations of atomistic systems. Such potentials are constructed by fitting large data sets from electronic structure calculations using machine learning (ML), thereby providing the accuracy of first principles calculations and the efficiency of simple atomistic force-fields. Despite the advent of fast computers and efficient algorithms, simulations of colloidal systems remain computationally challenging as very different length and time scales are involved. Huge efforts have been devoted to speeding up simulations of these systems by using coarse-grained (CG) models with effective interaction potentials, which are based on an ad-hoc parameterization to match reference data. However, the so-obtained potentials inevitably suffer from transferability and representability issues. In this work, we use ML to construct accurate and transferable CG many-body potentials for a variety of complex colloidal systems, including colloid-polymer mixtures and anisotropic rod-like nanoparticles. In our approach, a set of degrees of freedom are formally integrated out and the colloidal particles interact with effective many-body potentials, which we fit as a function of all colloid coordinates (and orientations) using a set of descriptors of local environments. Our ML method reduces the computational cost by several orders of magnitude compared to simulations of the full or fine-grained systems, and accurately describes the phase behavior and structure.

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Poster 39

Mechanical response of an inhomogeneous glass obtained via thermal processing

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A thermal gradient applied to a liquid mixture initiates transport processes resulting in a spatially non-uniform density and concentration profiles, in the steady state. Using extensive computer simulations, we study the response of a glassy mixture exposed to a thermal gradient, while we change the ambient temperature and quantify the extent of spatial heterogeneities that develop, both in the liquid and glassy regime. Subsequently, we study the shear response of such thermally processed glassy samples, over a range of shear-rates. We observe the emergence of non-equilibrium steady states depends upon the thermal processing. Consequently, that affects the formation of shear-bands in the transient regime.

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Poster 40

Microscopic origin of excess wings in relaxation spectra of supercooled liquids

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Glass formation is encountered in diverse materials. Experiments have revealed that the dynamic relaxation spectra of supercooled liquids generically become asymmetric near the glass transition temperature T_g , where an extended power law emerges at high frequencies. The microscopic origin of this 'wing' remains unknown, and has so far been inaccessible to simulations. Here we develop a novel computational approach and study the equilibrium dynamics of model supercooled liquids near T_g . We demonstrate the emergence of a power-law wing in the numerical spectra, which originates from relaxation at rare, localized regions over broadly distributed timescales. We rationalize the asymmetric shape of the relaxation spectra by constructing an empirical model associating heterogeneous activated dynamics with dynamic facilitation, which are the two minimal physical ingredients revealed by our simulations. Our work offers a glimpse into the molecular motion responsible for glass formation at relevant experimental conditions.

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Poster 41

MIPS beyond simple repulsive interactions

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Among active matter phenomena, motility-induced phase separation (MIPS), which leads to condensed active matter in the absence of cohesive forces, is a paradigmatic example of how activity overcomes the constraints imposed in equilibrium. MIPS starts to be well understood for self-propelled spherical particles interacting via purely repulsive forces. Its interplay with other interactions, from attractive tails to aligning torques, leads to a rich physics that we illustrate with numerical simulations. We then show how a generalized stress tensor formalism accounts for MIPS in the presence of these more general interactions, accounting both for re-entrance phenomena as well as alignment-induced MIPS.

Poster 42

Molecular DFT for solvation properties - beyond HNC

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The solvation properties of molecules or macromolecules immersed in various solvents, mainly water, are considered within the DFT approach in its molecular version. The systematic use of expansions/projections of angular functions onto rotational invariants (generalized spherical harmonics) greatly simplifies and accelerates the calculation of the OZ rotational convolution products and make it possible to solve "1D" codes (1 solute-solvent distance and 5 Euler angles for the solute+solvent orientations) or "3D" codes (3 spatial coordinates + 3 Euler angles for the solvent around a fixed solute) in a few minutes for any molecular or macromolecular solute [1]. Up to now, the approach has been restricted to the HNC level of approximation. Comparison with reference simulation data in terms of solvent density profile and solvation free energy indicates that the solute-solvent bridge functions b ignored by HNC are somewhat missing in the case of water solvent [2]. The present study investigates different routes for improving the closure or functional and deriving robust approximations for b . Some follow the WDA (Weight Density Approximation) approach [3], others the BHP approximation for the three-body direct correlation function, proposed by Barrat, Hansen, Pastore in 1988 [4].

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Poster 43

Negative thermal expansion in liquid covalent alloys

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The Peierls distortion is a spontaneous symmetry breaking mechanism that ultimately is responsible for the celebrated octet rule. Moreover, a Peierls-like distortion may exist in some covalent liquids, as it has been proven experimentally e.g. in liquid As [1]. Indeed, the chemical bond is primarily a local property and is similar in crystals, amorphous or liquid matter. Some liquid covalent alloys show a negative thermal expansion (NTE). Most of them are tellurium compounds. Based on a simple tight-binding approach, we analyse the vibrational properties of liquid alloys at the vicinity of the

Peierls transition. They show an anomalous behaviour that leads to a negative Grüneisen coefficient and ultimately to a NTE, in most cases just above the melting temperature or in the supercooled liquid. We finally analyse the existence and conditions of a liquid-liquid phase transition

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Poster 44

Networks of patchy colloidal platelets

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Colloids with localized bonding sites, commonly referred to as patchy particles, have sparked a considerable amount of interest for their ability to form equilibrium gels at low density [1]. In two dimensions, these low density colloidal gels are porous monolayers that can be utilized for filtration at the nano- and microscale as well as for optical applications, where their disordered nature may even support the formation of a material with a full photonic gap [2]. In this computational work, we study the properties and formation of two-dimensional gel networks from regular rhombic platelets decorated with four patches [3]. We find that by gradually varying the patch placement on the platelet edge as well as by switching the arrangement of the patch types, we can control the geometric properties of the forming networks such as local bonding motives, typical pore sizes and shapes, as well as branch-thickness. It is interesting to note that for all variations of these patch parameters, the location of the percolation line, the network connectivity as well as the network degree remained comparable.

We are convinced that further study of networks formed by anisotropic particles will lead to the discovery of novel network topologies that may be utilized for applications at the nano and micro scale.

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Poster 45

Obtaining dilute ferromagnetic frozen structures from the dipolar hard sphere fluid

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The study of magnetic nanoparticles (MNP) assembled in superstructures is an active field in nanomagnetism because of their potential applications and fundamental interest. The theoretical modelling of their properties is all the more important that the progress in experimental synthesis leads to an increasing variety of such superstructures, organized or not in large scale supracrystals. In these superstructures, the high concentrations in MNP lead to collective behaviors between MNP magnetic moments and complex magnetic phases (ferromagnetic or spin-glass) are expected at low temperature. Small enough MNP fall in the single domain regime and thus can be modelled in the framework of effective one spin (or macro-spin) models, i.e. ensembles of spherical particles bearing

a constant magnetic moment interacting through the dipole-dipole interaction (DDI) and a short range potential and undergoing the magnetocrystalline anisotropy (MAE).

The latter is a one-body potential imposing a preferential orientation for the moment on each MNP, the easy magnetization axis, and is characterized by the easy axis distribution, $\{\hat{n}_i\}$, and the coupling, λ_u . When the short range potential describes only the steric effects through the hard-sphere potential, one is left with the dipolar hard sphere fluid (DHS) at least in the absence of MAE or in the liquid state (ferro fluid) if one considers that the MNP being free to rotate, the easy axes follow instantaneously the moments. Both the DHS at sufficiently high volume fraction [1] and the ensemble of frozen dipoles on a perfect lattice of FCC or BCT symmetry order at low temperature in a well defined FM phase [2]. This is also the case for a frozen hard sphere like distribution of particles at a volume fraction larger than $\Phi_s = 0.495$ [3]. At lower packing fractions, the FM order is destroyed and instead a SG phase takes place.

In this presentation, we show that the FM ordering can be restored at lower densities by considering frozen structures derived from the DHS. Two values of the volume fraction, $\Phi = 0.45$ and 0.26 for which the DHS presents a PM/FM transition at a critical temperature $T_c(\Phi)$ are taken as examples. The frozen structures are derived from the DHS taken at temperatures T_f lower than the corresponding $T_c(\Phi)$. We first characterize the spatial anisotropy of the dipolar hard spheres configurations taken from the ferromagnetic liquid states then we determine the magnetic phase diagram in the (T, T_f) plane, where T_f is understood as an intrinsic disorder control parameter. We show that even at $\Phi < \Phi_s$ the system orders in a well defined FM phase for $T_f < T_c(\Phi)$.

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Poster 46

Osmolytes and electrolytes: bio-electrostatics through the lens of halophilic organisms

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Cellular functionality relies on the ability to maintain protein structure and function, and of significance to the latter is the ability of a protein to effectively find its binding site on a partner protein amid a crowded cellular environment. These interactions rely on finely tuned contributions to the overall force, including long-range electrostatic repulsion from a net-negative charge on a protein surface, along with attractive dispersion forces and more specific short-range interactions. The medium surrounding proteins in the cell – the cytosol – plays a vital for this fine tuning, and as a result it is puzzling how protein structure and function can be maintained across a wide range of cytosolic compositions and concentrations found across the spectrum of life. Nowhere is this clearer than in the case of the halophilic organisms: the single-celled organisms that accumulate high levels of osmolytes, components that range from simple salts to larger molecules, both ionic and non-ionic, in response to the high ionic strength of the growth environment.

In order to probe the role of osmolytes in maintaining protein functionality, we have performed model surface force measurements on simple osmolyte mixtures confined between two planar, charged sheets in order to afford molecular-level resolution. We found that presence of the common osmolyte trimethylglycine strongly influences the interaction potential between two mica sheets in multiple, distinct ways, including: it increases the strength and range of electrostatic repulsion, it disrupts water structure, and, in greater concentrations can form its own molecular layers at the charged surfaces.

We propose that osmolytes' role in maintaining protein stability is via multifaceted contributions to both the interaction potential and molecular organisation at charged surfaces.

Poster 47

Overlap and glass quantization of the Gaussian core model

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Systems of ultrasoft particles exhibit complex liquid-solid phase diagrams. In order to study the dynamical glass transition occurring within these systems, we use the replica method, involving two identical copies, conjugated with classical integral equation theories of the liquid state, focusing on low temperatures and low-to-moderate densities. For particles interacting through the Gaussian Core Model, we demonstrate that at constant temperature, a "continuous" glass state is entered upon a first compression but this glass melts as the density is further increased. In addition to this reentrant transition, a second, transition is discovered at higher densities between the "continuous" glass and a quantized glass. The overlap Q (i.e. the order parameter of the transition) of the former is a continuous function of temperature, while Q of the latter exhibits a succession of stripes. The glass physics of ultrasoft particles is hence richer than that of impenetrable particles.

Poster 48

Phase separation in an approximate equilibrium model of active matter: a transition driven by multibody interactions

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Remarkably, self-propelled particles are able to phase separate in spite of interacting via pairwise repulsive short-range forces. It is well-known that, at the two-particle level, the interplay between persistent self-propulsion forces and repulsive interactions leads to an effective attraction. At the many-body level, the stationary distribution deeply differs from that of simple fluids in equilibrium whose constituents also interact via pairwise forces. Indeed, the knowledge of the pair distribution function in a two particle system is simply not enough to qualitatively predict the stationary phase diagram. This is clearly identified in a recent work by Turci & Wilding, where effective multibody interactions were shown to be of paramount importance to account for the phase separation of self-propelled particle systems interacting via repulsive pairwise forces.

In this presentation, we provide an analytical picture for why the two-body effective attraction cannot account on its own for the observed phase separation. We then illustrate, within the unifold colored noise approximation, and within a controlled mean-field setting, the role of effective multibody interactions in shaping the phase behavior.

Poster 49

Phase transitions on non-uniformly curved interfaces: migrating matter

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In uniform three-dimensional space and flat two-dimensional space, the various states of matter can exist anywhere because of the translational and rotational invariance of space. In two dimensions, the introduction of uniform curvature (as on the surface of a sphere) can strongly affect structure, phase transitions and dynamics of particles confined to the surface [1-3], but all locations are still equivalent. In contrast, on non-uniformly curved surfaces, different states of matter may have structural or thermodynamic preferences for regions of different curvature [4]. Hence, phase transitions may be accompanied by the cooperative migration of matter to a new position [5].

We show how specially designed simulations can be used to investigate this coupling of phase and location for model colloidal clusters on toroidal and sinusoidal surfaces. The observations can be rationalised and quantified in terms of three universal, competing effects: cluster perimeter, stress and nearest-neighbour packing. We predict that migration at phase transitions could arise in any non-uniformly curved soft-matter system, including simple spherical colloids. It is also possible for the coupling between phase and location to result in additional (meta)stable states with order that is intermediate between liquids and crystals [5].

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Poster 50

Polymers under electroosmotic flow: insight from mesoscopic simulations

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Progress in the manufacturing of microfluidic and even nanofluidic devices has opened new avenues for manipulating the flow of fluids through complex environments. A major objective of research in nanofluidics is to achieve a better selectivity in manipulating the fluxes of nano-objects, and in particular of biopolymers.

Our focus here is polymer flows in confinement, which are subject to the simultaneous influence of intermolecular forces, thermal fluctuations, solvent-induced hydrodynamics and electric charge from the confining walls. Numerical simulations allow one to better understand the physical mechanisms at play in such situations. We performed hybrid mesoscale simulations to investigate the properties of polymers under flows in slit pores, at the nanoscale. We use multiparticle collision dynamics, an algorithm that includes hydrodynamics and thermal fluctuations. We investigate the properties of fully flexible and stiff polymers under several types of flow, and we show that Poiseuille flows and electro-osmotic flows can lead to quantitatively and qualitatively different behaviors of the chain.

In particular, a counter-intuitive phenomenon occurs in the presence of an electro-osmotic flow: When the monomers are attracted by the solid surfaces through van der Waals forces, shear-induced forces lead to a stronger repulsion of the polymers from these surfaces. Such focusing of

the chain in the middle of the channel increases its flowing velocity, a phenomenon that may be exploited to separate different kinds of polymers.

Poster 51

Position-dependent memory kernel in generalized langevin equations: theory and numerical estimation

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Generalized Langevin equations with non-linear forces and position-dependent linear friction memory kernels, such as commonly used to describe the effective dynamics of coarse-grained variables in molecular dynamics, are rigorously derived within the Mori-Zwanzig formalism. A fluctuation-dissipation theorem relating the properties of the noise to the memory kernel is shown. The derivation also yields Volterra-type equations for the kernel, which can be used for a numerical parametrization of the model from all-atom simulations.

Poster 52

Revealing supraparticle structure using unsupervised machine learning

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Rapid developments in machine learning (ML) have opened the door to unprecedented ability to autonomously detect structural variations in colloidal self-assembled systems. This includes even identifying different local structural features in systems generally thought of as disordered – for instance, glassy materials. However, identifying the intricate structure in colloidal supraparticles turns out to be even more challenging. Consider, for example the superstructure formed when, e.g. 10,000 hard spheres are self-assembled in spherical confinement – the resulting structure is an icosahedron, with an intricate arrangement of 3D face-centered-cubic domains, 2D domain walls separating these domains, and 1D domain edges. The challenge of autonomously extracting this superstructure turns out to be significantly more difficult than, e.g. distinguishing a crystal nuclei forming in metastable liquid. Here we present an unsupervised machine learning algorithm, based on a variational autoencoder (VAE), that significantly improves our ability to autonomously extract local structural variations: we demonstrate that the VAE-based approach can identify complex structures in supraparticles self-assembled from binary mixtures of hard spheres. With this approach we are able to identify essentially all components of the supraparticle structure including bulk crystal domains (3D), domain walls (2D), domain edges (1D) and point defects (0D).

Poster 53

Shear and bulk acceleration viscosities in simple fluids

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Any fluid in motion generates a viscous response that offers resistance to changes in the magnitude and in the direction of the flow. Viscous phenomena appear in any type of flow, ranging from atomic to atmospheric and cosmic flows.

The viscous response dampens the inhomogeneities of the velocity field of the flow. The viscous force splits into bulk and shear contributions, which are associated with the divergence and the curl of the velocity field, respectively. Both bulk and shear contributions are well understood and play a central role in the widely-used Navier-Stokes formalism.

Here, we propose and demonstrate, using particle-based computer simulations, the existence of analogue viscous contributions but associated to the divergence and the curl of the acceleration field instead of the velocity field. Both the velocity and the acceleration fields are required to accurately describe the viscous response of a simple fluid microscopically and temporally resolved at the atomic scale.

Our findings apply to any rapidly changing flow. Therefore the acceleration contribution to the viscous force described here is significant for the quantitative description of a wide range of flows, including shock waves, turbulent flows, inertial microfluidics, and mudflows among others

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Poster 54

Simple fluid with broken time reversal invariance

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We present a system of hard spheres with a simple collision rule that breaks time reversal symmetry, yet conserves energy as well as mass and momenta. It leads to an isotropic homogeneous stationary state. In this nonequilibrium fluid state correlated velocities emerge, a known phenomenon from active particles. They are long-ranged decaying like $1/r^d$ in d dimensions. Such correlations are expected on general grounds but had previously been observed in driven systems only. Simulations are compared to an approximate theory originally developed for granular systems.

Poster 55

Spontaneous propulsion of an isotropic colloid in a phase-separating environment

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The motion of active colloids is generally achieved through their anisotropy, as exemplified by Janus colloids. Recently, there was a growing interest in the propulsion of isotropic colloids, which requires some local symmetry breaking. Although several mechanisms for such propulsion were proposed, little is known about the role played by the interactions within the environment of the colloid, which can have a dramatic effect on its propulsion. Here, we propose a minimal model of an isotropic colloid in a bath of solute particles that interact with each other. These interactions lead to a spontaneous phase transition close to the colloid, to directed motion of the colloid over very long timescales and to significantly enhanced diffusion, in spite of the crowding induced by solute particles. We determine the range of parameters where this effect is observable in the model, and we propose an effective Langevin equation that accounts for it and allows one to determine the different contributions at stake in self-propulsion and enhanced diffusion.

Poster 56

Spontaneous self-assembly of a tunable octagonal quasicrystal in hard spheres on a plane

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Hard spheres are one of the most fundamental model systems in soft matter physics, and have been instrumental in shedding light on nearly every aspect of classical condensed matter. However, to date, they have not proven useful in the study of quasicrystals. Here, I show that an extremely simple model system, consisting of two sizes of hard spheres resting on a flat plane, can self-assemble into two distinct quasicrystal phases. The first quasicrystal is a dodecagonal square-triangle tiling, commonly observed in a large variety of colloidal model systems. However, the second quasicrystal, with octagonal symmetry, consists of three types of tiles: triangles, small squares, and large squares, and to our knowledge has not been previously seen in soft matter systems. The relative concentration of the different tiles can be continuously varied by tuning the number of smaller spheres present in the system, and satisfies constraints that can be understood by considering the four-dimensional (lifted) representation of the quasicrystal lattice. Both quasicrystal phases form reliably and rapidly over a significant part of parameter space, suggesting that hard spheres on a plane are an ideal model system for exploring quasicrystal self-assembly on the colloidal scale.

Poster 57

Stress and forces in scalar active fluids

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Understanding and predicting the forces generated in fluids due to the presence of interfaces and surfaces are of interest for a wide range of applications including the interfacial tension between different phases and depletion forces acting on immersed bodies. I will present recent advances for scalar active fluids in which the non-aligning constituents are self-propelled [1], and how the stress can be used to predict phase equilibrium [2] and forces on non-symmetric bodies [3]. I will also show

recent experimental results for the depletion force between a probe and wall due to the surrounding active fluid [4].

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Poster 58

Structure and interactions in a water-in-salt electrolyte: interface and bulk

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Water-in-salt electrolytes are species that are able to dissolve in water such that the salt accounts for the majority of the mass and volume of the system [1]. A key feature of these electrolytes is their ability to form passivating films on battery electrodes in an aqueous medium, presenting the possibility of energy dense lithium-ion energy storage devices that utilise non-toxic and environmentally friendly water as a solvent [1,2]. Investigations using small-angle neutron scattering has revealed a long-range length scale in the bulk liquid corresponding to nano-heterogeneities of hydrophobic and hydrophilic domains [3]. Here we present surface force measurements combined with small- and wide-angle neutron scattering measurements of the water-in-salt electrolyte lithium bis(trifluoromethanesulfonyl)imide, to investigate the structure of these nano-heterogeneities in the bulk liquid and at interfaces. At interfaces, we observe oscillatory layering across a range of concentrations on the same length-scale as previously observed, which we attribute to a templated, layered structure of alternating hydrophobic and hydrophilic domains [3,4]. In the bulk liquid, we observe the same nano-heterogeneities and construct a 3D model of the system using empirical potential structure refinement. Our results show the complex structures adopted in these materials both at charged interfaces and in the bulk liquid, and will have consequences for the design of new batteries and supercapacitors, as well as for the understanding of highly concentrated electrolytes.

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Poster 59

Supercritical fluids in confinement: structure-dynamics correlation

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The correlations between the structure and dynamics of partially confined Lennard Jones fluids, deep into the supercritical phase, is investigated over a wide range of densities in the context of the Frenkel

line (FL), which separates rigid liquidlike and non-rigid gaslike regimes in the phase diagram of the supercritical fluids. While varying wall stiffness, soft walls lead to diminishing structural order, enhancing self-diffusion for liquidlike regime, in a sharp contrast to that of the gaslike regime, where the trend reverses. Pair-excess entropy seems to capture this peculiarity in structure-dynamics correlations. Further, assessing FL crossover using density of states (DoS) function, supercritical fluids are seen to exhibit a progressive shift of FL crossover at higher temperatures for smaller spacings. These observations open up and attempt to understand the complexity of the interplay between structure and dynamics in confined liquids above critical point.

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Poster 60

The influence of confinement on the self-assembly of colloidal systems with competing interactions

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Systems with competing interactions, such as mixtures of surfactants, diblock copolymers and colloids, are important in industry, technology and biology. Although these systems have a different chemical identity, their phase diagrams exhibit the same topology in bulk. Cluster-crystals, hexagonal cylindrical, cubic triply periodic and lamellar phases have been observed in all those systems. We study the behaviour under confinement of colloidal particles interacting via short-range attraction and long-range repulsion (SALR) using Grand Canonical Monte Carlo (GCMC) simulations. We found that the confinement into pores of different geometries can significantly change the morphology of the bulk phases. In particular, we observe the formation of different helical structures in cylindrical pores [1] and cluster-crystals, that are not stable in bulk, in three-dimensional ordered pores [2]. On the other hand, we found that confinement can also favour the formation of phases with the same symmetry of those in bulk [2,3]. We believe that these findings can inspire experimental studies and contribute to the development of new functional materials.

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Poster 62

The phase transition of nearly hard spheres

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Classical theories of simple liquids, relying on mapping to hard spheres, have proven successful for purely repulsive systems such as the Weeks-Chandler-Andersen (WCA) model [1]. Here, we compute the solid-fluid coexistence line of the WCA model to high precision by combining the interface pinning method [2] and Kofke's Gibbs-Duhem integration method. The calculated line covers more than four decades of temperatures and focuses on the low-temperature limit where the WCA particles are nearly hard spheres. This accurate determination of the phase transition line allows for a critical review of theories mapping repulsive systems to hard spheres. Specifically, we

investigate classic criteria for effective hard-sphere diameters suggested by Andersen-Week-Chandler, Barker-Henderson, and Boltzmann. We present a new analytical prediction based on the isomorph theory of freezing [3, 4] and show that it gives better predictions than the classical hard-sphere theories.

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Poster 63

The role of interactions on the frequency-dependent conductivity of electrolyte solutions: insights from Brownian dynamics simulations and stochastic Poisson-Nernst-Planck theory

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Recent advances in nanoscale electrochemistry promise applications such as high performance batteries or ultra fast and accurate sensing in biological systems [1,2], but understanding the underlying dynamics remains a crucial step to control the transport of matter at the nanoscale [3], which play a fundamental role in these applications. The dynamics of ions in the presence of time-dependent electric fields is one of the central problems in physical electrochemistry. For example, the conductance of aqueous electrolyte solutions displays a generic $1/f$ noise at low frequencies [4], repeatedly observed in nanopores [5,6,7], yet a full explanation of its origin and its dependence on the physical and chemical properties of the pores remains elusive. Here we investigate the effects of several of such factors that may play a role on ionic current fluctuations: the confinement by the walls, surface charge, as well as steric and electrostatic interactions between ions.

Using Brownian dynamics simulations [8] of a bulk and confined implicit-solvent binary electrolyte, we study equilibrium structural and dynamical properties arising from the above-mentioned interactions. From there, we use linear response theory for Brownian dynamics [9] to compute the effective frequency-dependent conductivity of the system ranging over several orders of magnitude (from 10 MHz to 1 THz), and compare the simulation results to analytical predictions from stochastic Poisson-Nernst-Planck theory [10,11]. Brownian dynamics simulations allow to explore considerably longer time scales than molecular dynamics, while conserving sufficient details to understand macroscopic properties of confined ionic transport from simple microscopic interactions, and to go beyond the approximations of the mean-field analytical theories limited to low concentrations.

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Poster 64

Thermodiffusion and thermo-osmosis in porous media

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When a temperature difference is applied over a porous medium soaked with a fluid mixture, two effects may be observed, a component separation (the Ludwig-Soret effect, thermodiffusion) and a pressure difference due to thermo-osmosis. In this work, we have studied both effects using non-equilibrium thermodynamics and molecular dynamics. We have derived expressions for the two characteristic parameters, the Soret coefficient and the thermo-osmotic coefficient in terms of phenomenological transport coefficients, and we show how they are related. Numerical values for these coefficients were obtained for a two-component fluid in a solid matrix where both fluid and solid are Lennard-Jones/spline particles. We found that both effects depend strongly on the porosity of the medium and weakly on the interactions between the fluid components and the matrix. The Soret coefficient depends strongly on whether the fluid is sampled from inside the porous medium or from bulk phases outside, which must be considered in experimental measurements using packed columns. If we use a methane/decane mixture in bulk as an example, our results for the Soret coefficient give that a temperature difference of 10 K will separate the mixture to about 49.5/50.5 and give no pressure difference. In a reservoir with 30 % porosity, the separation will be 49.8/50.2 whereas the pressure difference will be about 15 bar. Thermo-osmotic pressures with this order or magnitude have been observed in frost-heave experiments.

Poster 65

Topological defects and the melting in two dimensions

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Topological defects have a preponderant role in the physics of (quasi) two-dimensional systems. One of the first applications is the description of the XY model by Kosterlitz and Thouless in the 1970s; this theoretical description of the XY model made possible in the 1980s to formulate a theory for the fusion in two dimensions, the KTHNY theory (Kosterlitz - Thouless - Halperin - Nelson - Young). In KTHNY, the transition from the solid phase to the liquid phase occurs with an intermediate phase, the hexatic phase, and each of the transitions: solid/hexatic and hexatic/liquid is of the KT type.

The microscopic mechanisms in KTHNY leading to phase transitions are dissociations of clusters of topological defects: the dissociation of dislocation pairs into free dislocations (solid/hexatic) and the dissociation of dislocations into free disclinations (hexatic/liquid). This description of the two-dimensional melting is in competition with a first-order transition between solid and liquid, without hexatic phase.

The existence of an intermediate hexatic phase for simple systems in two dimensions remained hypothetical until the mid-2000s when it was observed in experiments on superparamagnetic colloids confined to a water-air interface [1]. This observation reinforces the relevance of KTHNY theory. Then, with computer simulations of hard disks [2] and in colloidal systems [3], the hexatic/liquid transition is found to be first order, not predicted by the KTHNY theory.

In this contribution, we show that the mechanisms of dissociation of the KTHNY topological clusters are responsible for the solid/hexatic and hexatic/liquid transitions, and that, by a statistical analysis of the topological clusters, the KTHNY theory is compatible with a first order transition for the hexatic/liquid [4,5].

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Poster 66

Towards a microscopic understanding of underscreening in concentrated electrolytes: from bulk to confinement

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Electrostatic interactions play a critical role from biological systems to energy materials [1,2]. The classical Debye-Hückel and mean-field theories provide fundamental understandings of the screening of ionic interactions, but their applicability is limited only to dilute electrolytes [3,4]. Recent surface force measurement experiments [5,6] have challenged our current understanding of the screening phenomena: various concentrated electrolytes confined by mica surfaces show an unexpectedly long decay length of the force between surfaces (~ 10 nm), referred to as “underscreening”. Furthermore, they exhibit a universal cubic scaling relation of the decay length with ion size after properly normalizing both quantities with Debye screening length. Since the decay at large distance of the force between surfaces is expected to reflect the bulk correlation length of the liquid [6], several groups employed liquid-state theories or simulations to investigate bulk concentrated electrolytes. However, the anomalous underscreening found in the experiments is still puzzling, as bulk theories with the primitive model of electrolytes [7] and all-atom simulations [8,9] have only found underestimated exponents (1-2) instead of the cubic scaling exponent. A similar conclusion was obtained using classical Density Functional Theory for the primitive model [10] or all-atom simulations [11] to predict the decay of the ionic density profiles near an interface. This poster presents our current efforts to understand the microscopic origin of the long decay observed in surface force measurements with concentrated electrolytes, mainly focusing on the effects of confinement and interfaces. As a key component missing in previous simulations, our confined electrolytes are modeled being in contact with the bulk reservoir so that their salt concentration varies under different confinement while maintaining constant chemical potentials. Such grand-canonical simulations are computationally feasible via a hybrid non-equilibrium MD/MC method [12], which we have implemented in LAMMPS, a widely-used open-source simulator. This work is a part of the SENSES (making Sense of Electrical Noise by Simulating Electrolyte Solutions) project [13], funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 863473)

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Poster 67

Understanding a protic ionic liquid at a charged interface

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Room temperature ionic liquids are often considered as concentrated electrolytes as they are solvent-free liquid with pure ions. Their applications have been widespread in areas such as energy storage, solvent extraction, and carbon dioxide capture. Although their applications are expanding, their properties, in particular, their interfacial properties are not well understood. In energy storage, ionic liquids have been explored to replace the traditional solid dielectric capacitors. It is therefore important to understand their electrical properties near the electrode-electrolyte interface where most of the electrical exchange occurred. The electrode-electrolyte interface with dilute electrolytes is well established. Therefore, we chose to study the electrode-electrolyte interface with a protic ionic liquid, ethylammonium nitrate (EAN), in water at different concentrations. In this work, we employed force measurement with surface force balance, electrochemical impedance spectroscopy and chronoamperometry/coulometry to explore the electrode-electrolyte behaviour at the gold-EAN interface from dilute to pure ionic liquid.

Poster 68

Wetting transition of active Brownian particles on a thin membrane

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We study non-equilibrium analogues of surface phase transitions in a minimal model of active particles in contact with a purely repulsive potential barrier that mimics a thin, porous membrane. Under conditions of bulk motility-induced phase separation, the interaction strength ϵw of the barrier controls the affinity of the dense phase for the barrier region. We uncover clear signatures of a wetting phase transition as ϵw is varied. In common with its equilibrium counterpart, the character of this transition depends on the system dimensionality: a continuous transition with large density fluctuations and gas bubbles is uncovered in 2d while 3d systems exhibit a sharp transition absent of large correlations.

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7. Additional Information

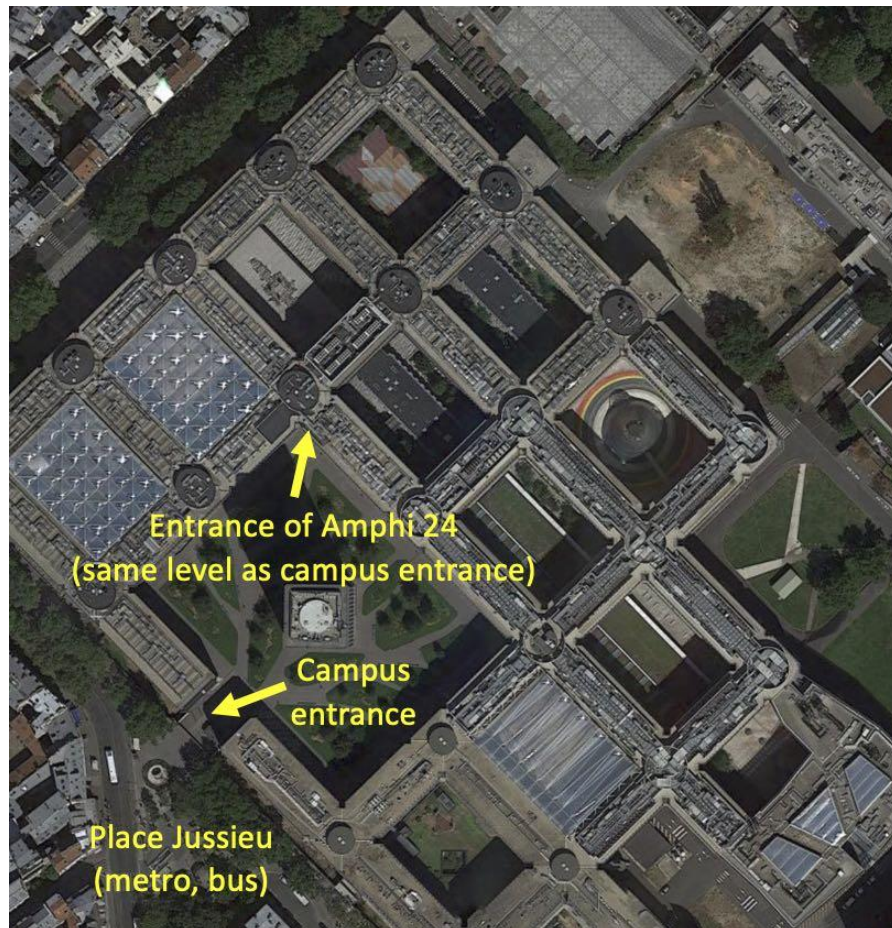
CECAM website for this workshop:

<https://www.cecarn.org/workshop-details/1111>

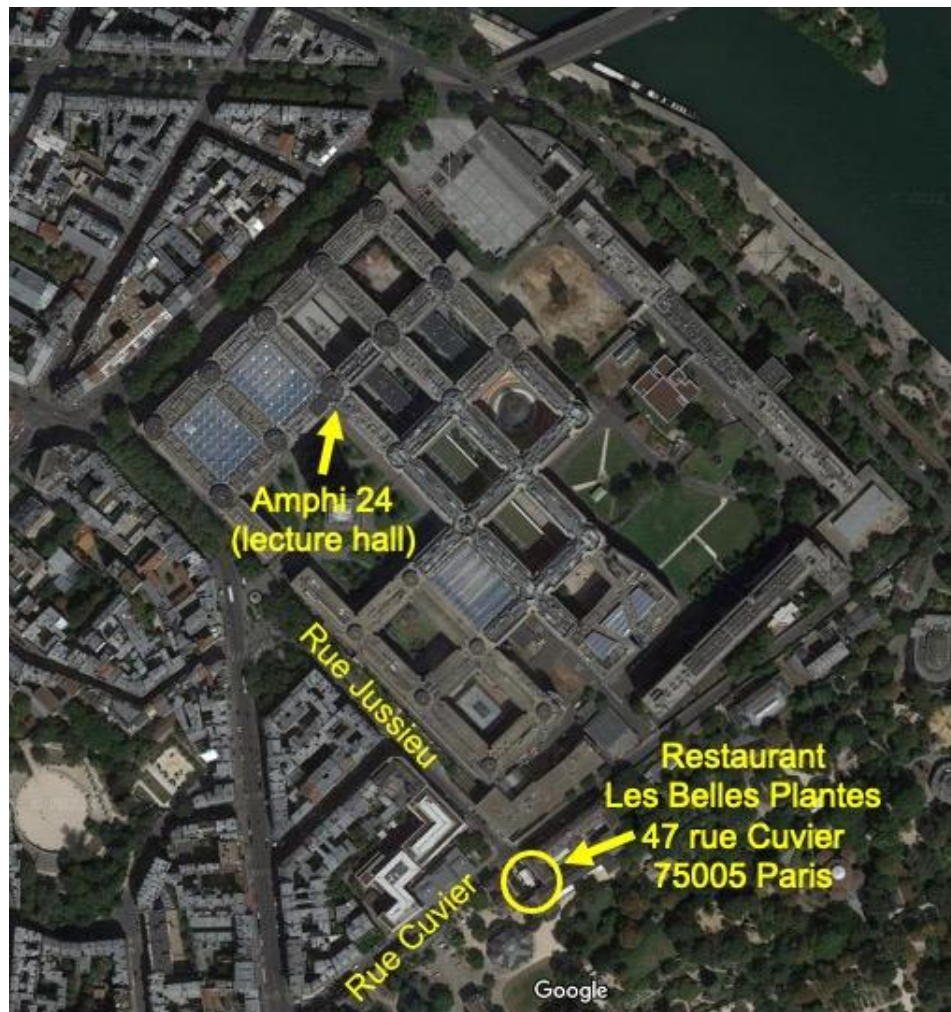
Download the Planify app:

8. Maps

Site of the Workshop



Restaurant (Dinner, July 6th, 2022)



9. Sponsors

