Wetting and Capillarity in Complex Systems

707. WE-Heraeus-Seminar

24 – 29 November 2019
at the Physikzentrum Bad Honnef/Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 707. WE-Heraeus-Seminar:

Wetting and capillarity phenomena are ubiquitous in nature, appearing in a variety of biological, physical, chemical and man-made systems, with applications which range, e.g., from microswimmers to the design of superhydrophobic surfaces. This seminar covers the emerging field of wetting in complex systems, where the notion "complex" applies either to the substrate, the liquid, or to the interaction between the two. In particular, understanding wetting processes in complex systems is key to manipulate and to control the behavior of simple and complex fluids, such as liquid crystals, ionic liquids, active fluids, polymers, via chemically and topographically controlled structured substrates.

The goal of the seminar is to achieve a "cross-fertilization" of ideas, understanding, and approaches between scientists who are working in diverse areas including Physics, Physical Chemistry, and Materials Science, all sharing an interest in wetting and capillarity. The seminar brings together a number of internationally recognized experts and young researchers who are using complementary methods — experimental, analytical, or simulation ones in order to address a number of issues which are important from both fundamental and practical viewpoints. More specifically (but not exclusively), the seminar will focus on four types of "complex systems":

- Wetting of and flow on structured surfaces
- Wetting by complex fluids such as colloidal suspensions, emulsions, liquid crystals, ionic liquids, electrolytes, polymers
- Active interfaces: microswimmers, active colloids, reactive wetting, responsive surfaces
- Colloids at fluid interfaces

Scientific Organizers:

Prof. Siegfried Dietrich	MPI für Intelligente Systeme and U Stuttgart, GER E-mail: dietrich@mf.mpg.de
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Program

Program

Sunday, 24 November 2019

17:00 – 20:00	Registration	
18:00	*BUFFET SUPPER and get-together*	

Monday, 25 November 2019

07:30	*BREAKFAST*	
08:45 – 09:00	Siegfried Dietrich	**Official opening and presentation of the seminar**
09:00 – 09:45	Thierry Ondarçuhu	**Dynamics of nanomenisci investigated by atomic force microscopy**
09:45 – 10:30	Hajime Tanaka	**A novel physical mechanism of liquid flow slippage on a solid surface**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Anton Darhuber	**Liquids with a sunburn: Marangoni flows induced by photochemical reactions**
11:45 – 12:30	Ofer Manor	**Transitions between different motion regimes of the three-phase contact line (and a newly found state of contact line motion) during the pattern deposition of polymer from a volatile solution**
12:30 – 12:40	**Conference Photo** (in the front of the lecture hall)	
12:40	*LUNCH*	

Program

Monday, 25 November 2019

14:30 – 15:15	Jacco Snoeijer	**Soft wetting: drops on elastic substrates**
15:15 – 16:00	Marek Napiórkowski	**Wetting of soft substrates**
16:00 – 16:30	*COFFEE BREAK*	
16:30 – 17:15	Alvaro Domínguez	**Active colloids near a responsive fluid interface**
17:15-18:00	Mihail Popescu	**Effective interactions between chemically active particles and walls**
18:45	*DINNER*	

Program

Tuesday, 26 November 2019

08:00	*BREAKFAST*	
09:00 – 09:45	Vinothan Manoharan	**Braiding micro- and nano-scale wires using capillary forces**
09:45 – 10:30	Rudi Podgornik	**General formulation and some salient results in charge regulation theory**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	David Andelman	**Going beyond the Poisson-Boltzmann theory: Interfacial properties and charge regulation of electrolytes**
11:45 – 12:30	Clarissa Schönecker	**Flow and slip measurements in extreme vicinity of structured surfaces**
12:30	*LUNCH*	
14:00 – 17:00	**Flash-Presentation + Poster-Session**	
	incl. COFFEE BREAK	
17:00 – 17:45	Jens Harting	**Capillary and electrostatic interactions in multiphase flows**
17:45 – 18:30	Robert Evans	**Molecular theory of capillarity: what we know now that Mr. Frumkin & Mr. Derjaguin did not know.**
18:45	*DINNER*	

Program

Wednesday, 27 November 2019

08:00	*BREAKFAST*	
09:00 – 09:45	Clemens Bechinger	**Cohesive swirls formed by active colloids**
09:45 – 10:30	Holger Stark	**Active particles: Capillary condensation and learned navigation**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Carlo Massimo Casciola	**A mesoscale model for liquid-vapor phase transition over solid surfaces**
11:45 – 12:30	Svyatoslav Kondrat	**Fluid-mediated interactions between colloids in bulk and confinement**
12:30	*LUNCH*	
14:30 – 18:00	**Excursion**	
18:45	*DINNER*	

Program

Thursday, 28 November 2019

08:00	*BREAKFAST*	
09:00 – 09:45	Lou Kondic	**Instabilities of liquid crystal films on nanoscale**
09:45 – 10:30	Felix Höfling	**Large-scale molecular dynamics simulations of inhomogeneous fluids: the boundary matters**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Margarida Telo da Gama	**Non-equilibrium interfaces of patchy colloids in 2 and 3D**
11:45 – 12:30	Catherine Barentin	**Wetting of yield-stress fluids**
12:30	*LUNCH*	
14:30 – 15:15	Sabine Klapp	**Taming bacterial turbulence by external fields and arrays of obstacles**
15:15 – 16:00	Lucio Isa	**Active colloids swimming at oil-water interfaces**
16:30 – 17:15	*COFFEE BREAK*	
16:30 – 17:15	Emanuela Zaccarelli	**Microgels at liquid-liquid interfaces**
17:15-18:00	Matteo Pierno	**Droplets dynamics from wall texturing to liquid surfaces**
18:00 – 18:15	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
18:45	*HERAEUS DINNER* *(social event with cold & warm buffet and complimentary drinks)*	

Program

Friday, 29 November 2019

08:00	*BREAKFAST*	
09:00 – 09:45	Hartmut Löwen	**Active particles near substrates: from biofilms to colloids in motility patterns**
09:45 – 10:30	Dirk Aarts	**Droplets of complex fluids on walls**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Serafim Kalliadasis	**Challenges of modelling the moving contact line problem and recent progress: bridging scales from the nano- to the macroscale**
11:45 – 12:30	Pierre Illien	**Experimental observation of flow fields around active Janus spheres**
12:30 – 12:40	Siegfried Dietrich	**Closing remarks**
12:45	*LUNCH*	

End of the seminar and departure

NO DINNER for participants leaving on Saturday morning

Posters

Posters

Shahriar Afkhami	**Pore-scale direct numerical simulation of Haines jumps in a porous media model**
Alejandro Avila-Sierra	**Surface wetting to cleaning-in-place optimisation**
Vincenzo Calabrese	**Charge-driven interfacial gelation of cellulose nanofibrils across the water/oil interface**
Rodrigo Coelho	**Propagation of interfaces in active liquid crystals on a substrate**
Sabyasachi Dasgupta	**From cellular to tissue mechanics: Fluidization based on topological activity**
Nicolò Giuseppe Di Novo	**Condensation frosting on nanostructured surfaces**
Raul Esquivel-Sirvent	**Theoretical study of liquid metal wetting**
Nima Farahmand Bafi	**Tricritical Casimir forces and order parameter profiles in wetting films of ^{3}He – ^{4}He mixtures**
David Feldmann	**Tuning the geometry of bioinspired biphilic surfaces for efficient water collection and transport**
Markus Gross	**Nonequilibrium dynamics of the critical Casimir force**
Florian Gußmann	**A MC-optimized DFT for the Jagla fluid**
Kirsten Harth	**Drop impact on hot plates: contact, rebound and the formation of holes**
Minkush Kansal	**Capillary instability of elastic solids**
Hyojeong Kim	**Interfacial wetting of binary liquid mixtures near a colloid**

Posters

Roland L. Knorr	**Intracellular wetting regulates degradation of fluid compartments**
Sergey Lishchuk	**Detachment work of prolate spheroids from fluid droplets**
Lidong Liu	**Capillary adhesive contact between soft microparticles**
Didier Long	**Wetting and dewetting of a nanoparticle at a polymer interface: numerical simulations based on a virtual work principle**
Anna Maciolek	**Wettability and illumination-induced motion of Janus particle**
Arghya Majee	**Electrostatic interaction of particles trapped at fluid interfaces: effects of geometry and wetting properties**
Suvendu Mandal	**Persistent correlations in colloidal suspensions**
Grégoire Martouzet	**Delayed dynamics of liquid droplet impact on multiscale super-hydrophobic surfaces**
Bortolo Matteo Mognetti	**Localized self-assembly triggered by functionalized interfaces**
Maximilian Mußotter	**Electrolyte solutions at heterogeneously charged substrates**
Piotr Nowakowski	**Membrane close to critical demixing with a single inclusion**
Gonçalo Paulo	**Synchronization in a binary mixture of brownian oscillators**

Posters

Christian Rohwer	**Non-equilibrium correlations and forces in sheared fluids with or without quenching**
Jose M. Romero-Enrique	**Wetting of nematic liquid crystals on crenellated substrates: a Frank–Oseen approach**
Peyman Rostami	**Capillary dynamics of a four-phase contact point**
Sutapa Roy	**Hot active Janus colloids in a binary solvent**
Artem Ryabov	**Plasma-assisted growth of polyethylene fractal nano-islands on polyethylene oxide thin films**
Andrew Salmon	**Artificial chromatophores: light-triggered nanoparticles for microdroplet locomotion and color change**
Lothar Schimmele	**Filling transitions of a partially miscible binary liquid on a nanosculptured surface**
Simon Schubotz	**Memory effects in polymer brushes showing co-nonsolvency effects**
Marion Lucia Silvestrini	**A study of metastability in hydrophobic surfaces**
Juliane Simmchen	**Hydrophobicity of surfaces in active matter**
Alessio Squarcini	**1. Action at a distance in classical uniaxial ferromagnetic arrays: exact results and wetting effects.** **2. The interface of the 3D Ising model and the vortex line in the 3D XY model: exact analytic results and numerical simulations.**
Paulo Teixeira	**The shape of liquid bridges**

Posters

Sumesh Thampi	**Dynamics of particles confined by droplets**
Antonio Tinti	**The triple line tension of water in extreme confinement**
Leon Topp	**Non-equilibrium effects of the wetting properties at switchable substrates**
Robin van Damme	**Hourglasses at a fluid-fluid interface: multipoles, demixing and hindered assembly**
Oleg Vasilyev	**Bridging transition between particles**
Binyu Zhao	**Surface wettability-induced sign inversion of the apparent line tension in sessile nanodroplets**

Abstracts of Talks

(in chronological order)

Dynamics of nanomenisci investigated by atomic force microscopy

C. Mortagne[1,2], K. Lippéra[2,3], M. Benzaquen[3], P. Tordjeman[1], T. Ondarçuhu[1,2]

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[2] CEMES-CNRS, Toulouse, France
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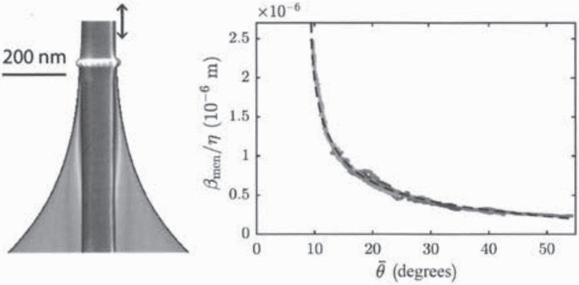
The ability to understand and control liquid flows and interface dynamics down to the nanometer scale is a major challenge in physics of liquids. Here, we show that atomic force microscope (AFM) used in dynamic mode, combined with the nanofabrication of dedicated tips ended by a nanocylinder allows quantitative measurements of the dynamics of nanomenisci. Monitoring the cantilever frequency-shift and the dissipation during the partial immersion of the nanofiber in a liquid, we study independently various contributions of the probe-liquid interaction, namely:

- the dissipation in the viscous layer around the fiber [1],
- the dissipation in the oscillating nanomeniscus (Figure) [2],
- the effective spring constant of the liquid interface [3].

These results show that AFM enables the accurate investigation of liquid flows down to the nanometer scale and open the way for the study of the dissipation associated with a moving contact line and its interaction with nanodefects [4].

[1] J. Dupré de Baubigny, M. Benzaquen, C. Mortagne, C. Devailly, J. Laurent, A. Steinberger, J.-P. Salvetat, J.-P. Aimé, T. Ondarçuhu, Phys. Rev. Fluids, 1 (2016) 044104.
[2] C. Mortagne, M. Benzaquen, K. Lippera, P. Tordjeman, T. Ondarçuhu, Phys. Rev. Fluids. Rapid Comm., 2 (2017) 102201(R).
[3] J. Dupré de Baubigny, M. Benzaquen, L. Fabié, M. Delmas, J.-P. Aimé, M. Legros, T. Ondarçuhu, Langmuir 31 (2015) 9790-9798.
[4] M. Delmas, M. Monthioux, T. Ondarçuhu, Phys. Rev. Lett. 106 (2011) 136102.



(a) Sketch of a nano-meniscus pinned on artificial defects deposited on a nanofiber (color: viscous stress);
(b) Dissipation in the nanomeniscus as a function of the contact angle.

A novel physical mechanism of liquid flow slippage on a solid surface

Hajime Tanaka and Yuji Kurotani

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Viscous liquids often exhibit flow slippage on solid walls, which apparently violates the so-called no-slip boundary condition [1-9]. The occurrence of flow slippage has a large impact on the liquid transport and the resulting energy dissipation, which are crucial for many applications. It is natural to expect that slippage takes place to reduce the dissipation. However, (i) how a liquid feels the presence of the wall and (ii) how it knows which pathway towards slippage to take to reduce the dissipation by forming a gas layer, remained elusive. Here we report the answers to these fundamental questions: (i) density fluctuation is intrinsically enhanced near the wall even in a quiescent state irrespective the property of wall and (ii) it is the density dependence of the viscosity [11,12] that destabilize the system toward liquid-to-gas transition under shear flow. Our shear-induced liquid-to-gas transition scenario provides not only a natural physical explanation for wall slippage of liquid flow, covering the slip length ranging from a microscopic (nm) to macroscopic (μm) scale, but also a way to intentionally prevent or induce it.

References

[1] C. Neto, D. R. Evans, E. Bonaccurso, H.-J. Butt, V. S. Craig, Rep. Prog. Phys. 68, 2859 (2005).
[2] E. Lauga, M. Brenner, H. Stone, Microfluidics: the no-slip boundary condition (Springer, New York, 2007).
[3] L. Bocquet, J.-L. Barrat, Soft Matter 3, 685 (2007).
[4] R. S. Voronov, D. V. Papavassiliou, L. L. Lee, Ind. Eng. Chem. Res. 47, 2455 (2008).
[5] L. Bocquet, E. Charlaix, Nanofluidics, from bulk to interfaces. Chem. Soc. Rev. 39, 1073 (2010).
[6] O. I. Vinogradova, Slippage of water over hydrophobic surfaces. Inter. J. Mineral Proc. 56, 31–60
[7] (1999).
[8] D. Ortiz-Young, H.-C. Chiu, S. Kim, K. Vo¨ıtchovsky, E. Riedo, Nature Commun. 4 (2013).
[9] R. Pit, H. Hervet, L. Leger, Phys. Rev. Lett. 85, 980 (2000).
[10] Y. Zhu, S. Granick, Phys. Rev. Lett. 87, 096105 (2001).
[11] A. Furukawa and H. Tanaka, Nature **443**, 434 (2006).
[12] A. Furukawa and H. Tanaka, Nature Mater. **8**, 601 (2009).

Liquids with a sunburn: Marangoni flows induced by photochemical reactions

J. Muller, H. M. J. M. Wedershoven, and A. A. Darhuber
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The Netherlands

We have studied flows of thin liquid film set up by photochemical reactions due to patterned illumination [1]. Light intensity gradients translate into gradients of the reaction products. The latter change the local surface tension and induce Marangoni flow in the liquid films. As a model system, we consider the irradiation of the aliphatic hydrocarbon squalane with broadband deep-UV light and use interferometry to detect the deformation of the liquid films. We developed a numerical model that quantitatively reproduces the flow patterns observed in the experiments. Moreover, we present self-similarity solutions that elucidate the mechanisms governing different stages of the dynamics and their parametric dependence.

We evaluated the sensitivity and time resolution of this technique for photochemical reaction monitoring. Surface tension changes as small as $\Delta\gamma = 10^{-6}$ N/m can be detected, and time resolutions below 1 s can be achieved.

References

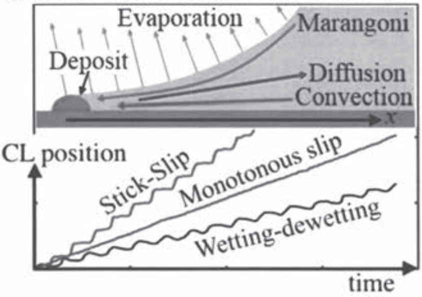
[1] J. Muller, H. M. J. M. Wedershoven, and A. A. Darhuber, Langmuir **33**, 3647 (2017)

Transitions between different motion regimes of the three-phase contact line (and a newly found state of contact line motion) during the pattern deposition of polymer from a volatile solution

M. Abo Jabal, A. Zigelman, and O. Manor

Chemical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

The motion of the three-phase contact line (CL) between a volatile solution, its vapor and a substrate, plays an essential role in the evaporative self-assembly (pattern deposition) of soft matter. We investigate the connection between the motion regimes of the CL of volatile polymer solutions and the deposit morphology. In particular, we report the mechanisms, which govern different motion regimes of the CL, e.g., monotonous slip and stick-slip motions. We further outline a newly found regime of CL motion, where the CL undergoes a periodic wetting/dewetting motion during solvent evaporation (see bottom of figure). This is the result of an unstable balance between contributions from solvent evaporation and Marangoni flow to CL motion. The former and later contributions support the dewetting and wetting of the substrate, respectively (see meniscus illustration at top of figure).



In our experiment, we evaporate solutions of Toluene and Poly-methyl-methacrylate or Poly-dimethyl-siloxane in micro-chambers, which support a linear CL geometry and a well-defined temperature and rate of evaporation [1]. We demonstrate that the regimes of CL motion and of polymer deposition may be anticipated when considering the balance between polymer diffusion and convection (which we quantify using a Peclet number) and the balance between evaporative and surface energy contributions to mass transport (which we quantify using a Marangoni number). Moreover, we use a long wave type theory to prove our assertions about the physics of the newly found regime of CL motion [2].

References

[1] M. Abo Jabal, et al., J. Colloids Interface Sci. **548**, 145-150 (2019)
[2] A. Zigelman, et al., Soft Matter **15,** 3580-3587 (2019)

Soft wetting: drops on elastic substrates

J.H. Snoeijer

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The laws of wetting are well-known for drops on simple rigid surfaces, but these change dramatically when the substrate is soft and deformable [1]. The combination of wetting and the intricacies of soft polymeric interfaces have provided many rich examples of fluid-structure interaction, both in terms of phenomenology as well as from the fundamental perspective. In this talk I will discuss experimental and theoretical progress on the statics and dynamics of soft wetting. In this context we critically revisit the foundations of capillarity, such as the nature of solid surface tension, the microscopic mechanics near the contact line, and the dissipative mechanisms that lead to unexpected spreading dynamics.

References

[1] B. Andreotti and J.H. Snoeijer, Annu. Rev. of Fluid Mech. **52**, (2020)

Wetting of soft substrates

M. Napiórkowski[1], L. Schimmele[2], and S. Dietrich[2,3]

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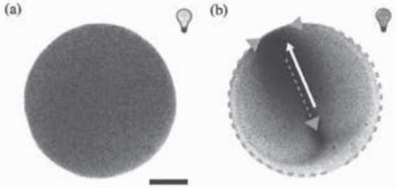
Within mean-field theory we study wetting of elastic substrates. Our analysis is based on a grand canonical free energy functional of the fluid number density and of the substrate displacement field. The substrate is described in terms of the linear theory of elasticity, parametrized by two Lamé coefficients. The fluid contribution is of the van der Waals type. Two potentials characterize the interparticle interactions in the system. The long-ranged attraction between the fluid particles is described by a potential $w(\boldsymbol{r})$, and $v(\boldsymbol{r})$ characterizes the substrate-fluid interaction. By integrating out the elastic degrees of freedom we obtain an effective theory for the fluid number density alone. Its structure is similar to the one for wetting of an inert substrate. However, the potential $w(\boldsymbol{r})$ is replaced by an effective potential which, in addition to $w(\boldsymbol{r})$, contains a term bilinear in $v(\boldsymbol{r})$. We discuss the corresponding wetting transitions in terms of an effective interface potential $\omega(\ell)$, where ℓ denotes the thickness of the wetting layer. We show that in the case of algebraically decaying interactions the elasticity of the substrate may suppress critical wetting transitions, and may even turn them first order.

ACTIVE COLLOIDS NEAR A RESPONSIVE FLUID INTERFACE

Alvaro Domínguez
Universidad de Sevilla, Spain

In the last years, man-made particles that alter their chemical environment (via catalytic activity) have become an easily acessible and controllable experimental system for addressing nonequilibrium phenomena. The most popular application has been the fabrication of self-propelled particles. A much less addressed manifestation of the chemical activity is the influence on nearby boundaries and the associated backreaction on the dynamics of the particles [1]. Here I address the case of a fluid interface with surface tension dependent on the local chemical environment: as a consequence, the chemical activity generates, regardless of self-propulsion, a *Marangoni flow* [2,3], which can become the driving force of the particle dynamics.

I will provide a brief discussion of the theoretical framework for the collective dynamics of active particles driven by the activity-induced Marangoni flow, together with some theoretical predictions [4,5]. I will also present the first experimental results ever that demonstrate this Marangoni-driven dynamics due to chemical activity: in this case, as an instance of spontaneous symmetry breaking [6] (see figure).



Droplet made of a colloidal dispersion (top view). *Left:* Homogeneous distribution at rest in the absence of chemical activity. *Right:* When the activity is turned on, the distribution becomes inhomogeneous and a steady flow pattern emerges. The scale bar corresponds to 100 μm.

References

[1] M. N. Popescu, W. E. Uspal, A. Domínguez, S. Dietrich, *Acc. Chem. Res.* **51**, 2991 (2018).
[2] H. Masoud and M. Shelley, *Phys. Rev. Lett.* **112**, 128304 (2014).
[3] A. Domínguez, P. Malgaretti, M. N. Popescu, S. Dietrich, *Phys. Rev. Lett.* **116**, 078301 (2016).
[4] A. Domínguez, P. Malgaretti, M. N. Popescu, S. Dietrich, *Soft Matter* **12**, 8398 (2016).
[5] A. Domínguez, M. N. Popescu, *Soft Matter* **14**, 8017 (2018).
[6] D. P. Singh, A. Domínguez, U. Choudhury, M. N. Popescu, S. Dietrich, P. Fischer, *submitted* (2019).

Effective Interactions between Chemically Active Particles and Walls

W.E. Uspal[1], M.N. Popescu[2], M. Tasinkevych[3], S. Das[2], and S. Dietrich[2]

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[2] *Max Planck Institute for Intelligent Systems, Stuttgart, Germany*
[3] *University of Lisbon, Lisbon, Portugal*

Chemically active particles can achieve force- and torque-free motility ("self-propulsion") via the promotion, on their surface, of catalytic chemical reactions involving the surrounding solution. The motion of such particles is intrinsically related to a "chemical field", i.e., the distribution of the number densities of the reactant and product chemical species present in the solution, and to the hydrodynamic flow of the solution around the particle. In most of the envisioned applications, and in virtually all reported experimental studies, the particles operate under spatial confinement (e.g., within a channel, a drop, or a free-standing liquid film). In such cases, the chemical field and the hydrodynamic flow associated with an active particle are influenced by any nearby confining surfaces, and these disturbances couple back to the particle. Thus, an effective interaction with the spatial confinement arises and, consequently, the particle is endowed with means to perceive and to respond to its environment.

We review the recent progress made, via simple models of chemical activity and self-phoretic motion, in understanding the basic physical principles of the complex behaviors induced by such effective interactions. First, we consider the occurrence of "interface-bounded" steady states of chemically active particles near "inert", i.e., no-slip walls. Examples include particles "sliding" along (or "hovering" above) a hard planar wall while inducing hydrodynamic flow of the solution [1-4]. These states lay the foundations for concepts like the guidance of particles by the topography of the wall. We then proceed to the case of "responsive" walls: a suitable chemical patterning of a planar wall allows one to bring the particles into states of motion which are spatially localized (e.g., within chemical stripes or along chemical steps) [3]. These occur because the wall responding to the activity-induced chemical gradients by generating osmotic flows, which encode the surface-chemistry of the wall.

References

[1] W.E. Uspal *et al*, Soft Matter **11**, 434 (2015)
[2] J. Simmchen *et at*, Nature Commun. **7**, 10598 (2016).
[3] W.E.Uspal *et at*, Phys. Rev. Lett. **117**, 048002 (2016); *ibid*, New J. Phys. **20**, 015013 (2018).
[4] S. Das *et al*, in preparation (2019).

Braiding micro- and nano-scale wires using capillary forces

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I will describe how capillary forces can be used to twist and braid micro- and even nano-scale wires. We attach such wires to polymer “floats” that reside at a water-air interface. These floats pin the contact line such that, when they are placed in a hydrophilic container, the capillary force between the floats and the container walls is repulsive. As a result, the floats—and therefore the wires—can be translated or rotated by moving the walls of the container. I will show how, by harnessing contact-line pinning, we can braid the wires simply by moving the interface up and down repeatedly.

This research is in collaboration with Cheng Zeng, John Miles Faaborg, Yohai Bar Sinai, and Michael P. Brenner at Harvard University.

General formulation and some salient results in charge regulation theory

R. Podgornik [12]

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There are no net charges in (bio)colloid world, and all of them result from dissociation of chargeable groups, as in e.g., proteins from dissociable amino acid moieties, a process in general referred to as charge regulation[1]. Recent advances in the theoretical formulation and analysis of charge regulated system lead to some far reaching conclusions on electrostatic interactions in colloid milieu, that often differ fundamentally from the accepted wisdom[2]. I will present several examples of novel behavior or new understanding of the known behavior that is specifically connected with the response of the charging equilibrium on (bio)colloidal surfaces to the local bathing solution conditions.

References

[1] R. Podgornik, The Journal of Chemical Physics **149**, 104701 (2018)
[2] Y. Avni, D. Andelman and R. Podgornik, Current Opinion in Electrochemistry, **13**, 70 (2019).

Going beyond the Poisson-Boltzmann Theory: Interfacial Properties and Charge Regulation of Electrolytes

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The Poisson-Boltzmann theory is a mean-field description of ionic solutions and electrified interfaces, and has been instrumental during the last century to predict charge distributions and interactions between charged surfaces, membranes, electrodes as well as macromolecules and colloids. While the electrostatic model of charged fluids, on which the Poisson-Boltzmann description rests, and its statistical mechanical consequences have been scrutinized in great detail, much less is understood about its probable shortcomings when dealing with various aspects of real physical, chemical and biological systems. After a short review of the Poisson-Boltzmann theory, I will discuss several modern extensions and modifications as applied to ions and macromolecules in confined geometries. They include among others the effect of dipolar solvent molecules, finite size of ions, ionic specificity and charge regulation of ionizable groups.

References

[1] Y. Avni, D. Andelman, R. Podgornik, Curr. Opin. Electrochem. **13**, 70 (2019).
[2] R. M. Adar, T. Markovich, A. Levy, H. Orland, D. Andelman, J. Chem. Phys. **149**, 054504 (2018).
[3] T. Markovich, D. Andelman, R. Podgornik, Europhys. Lett. **120**, 26001 (2017).
[4] T. Markovich, D. Andelman, R. Podgornik, Langmuir **33**, 34 (2017).

Flow and slip measurements in extreme vicinity of structured surfaces

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Structured surfaces lie at the core of many functional surfaces which may be employed for applications such as control of wetting, ant-biofouling, drag-reduction and many more. Geometric or sometimes even chemical structures at the nano- or micrometer level also cause the flow field to vary at this level. However, the details of the flow very close to surfaces are hard to determine, for example due to finite particles sizes in particle-based measurement techniques. Even with standard Fluorescence Correlation Spectroscopy (FCS), it is only possible to measure down to a distance of about 1 µm close to the surface. We therefore extended the standard FCS technique to distances below this limit. This was done by deriving a theoretical model that takes into account the immersion of the detection volume of the microscope into the surface. We applied this method to a superhydrophobic surface made from silicone nanofilaments. It is shown that a resolution of the flow at this level is indeed needed to correctly capture the high local slip length values that occur at these surfaces. The experiments are in good agreement with a simple numerical model of the surface. The simulations also show that possible gas slip of the air around the nanofibers has only a minor influence.

Capillary and electrostatic interactions in multiphase flows

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Colloidal particles adsorb to fluid-fluid interfaces and reduce the interfacial free energy which leads to an efficient interface stabilization. This effect is well known since the pioneering work of Pickering and Ramsden more than a century ago, but only recently scientists started to utilize tunable capillary interactions between adsorbed colloids to self-assemble complex structures for new soft and adaptive materials. We investigate the interplay of particle shape, contact angle, particle surface structure and external fields on the capillary assembly by means of hybrid lattice Boltzmann / molecular dynamics simulations and demonstrate how anisotropy in the geometry and wettability of colloidal particles can be utilized for the direct assembly of well-defined structures. The second part of the presentation summarizes recent results on electrokinetic effects in multiphase flows. We coupled our lattice Boltzmann solver to a solver for the Nernst-Planck equation. This allows us to resolve the coupled dynamics of several fluid and ion species. I will present first results ranging from floating droplets deforming in electric fields to electrowetting and the formation of ordered nanostructures in fluid mixtures with antagonistic salts.

Figure 1: Snapshot showing a time series of a charged droplet moving and breaking up in an electric field.

References

[1] Q. Xie, J. Harting, Langmuir **34**, 5303 (2018)
[2] Q. Xie, G. B. Davies, J. Harting, ACS Nano **11**, 11232 (2017)
[3] M. Wouters, O. Aouane, T. Krüger, J. Harting, Phys. Rev. E **100**, 033309 (2019)
[4] N. Rivas, S. Frijters, I. Pagonabarraga, J. Harting, J. Chem. Phys. **148**, 144101 (2018)
[5] D. Jung, N. Rivas, J. Harting, J. Chem. Phys. **150**, 064912 (2019)
[6] N. Rivas, J. Harting, arXiv:1805.01351 (2018)

Molecular Theory of Capillarity: what we know now that Mr. Frumkin & Mr. Derjaquin did not know.

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In this **Colloquium** I shall review some of the history of capillarity, wetting and surface phase transitions focusing on the development of microscopic theory and how this led to new statistical physics and to a host of experiments shedding fundamental new insight into fluid interfacial phenomena. I shall also describe some current work and look ahead to where investigations might be profitable.

Cohesive swirls formed by active colloids

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Many organisms form groups to protect from predators or optimize nutrient acquisition. Such collective states require individuals to permanently adjust their motion to neighbours which is explained by social attractive and aligning forces. Compared to swarms and flocks, swirls are predicted to be less stable and prone to noise and perturbations. This, however, seems in contradiction to the abundance of species, including fish, insects and even humans, being able to form collective rotating groups. Here, we experimentally demonstrate the formation of stable swirls in suspensions of light-responsive active colloidal particles which adjust their swimming direction by a simple rule to the positions and orientations of neighbours. We observe stable swirls which are not only robust against thermal noise but also to misbehaving individuals and obstacles. We expect our results to be relevant for the organization in biological and social systems and the design of scalable and autonomous micro-robotic systems.

Active particles: Capillary condensation and learned navigation

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Microswimmers move or need to navigate in complex environments such as porous soil or landscapes of external cues. The talk addresses two model situations of active particles in this respect.

First, I look at capillary condensation of a collection of active Brownian particles in a slit pore of varying width, which serves as a model pore [1]. Second, I address recent work where we look at optimal steering of active particles along the shortest path in a potential landscape and show how a smart active particle learns optimal steering via a reinforcement-learning strategy [2].

References

[1] M. Knežević and H. Stark, arXiv:1908.10483v1 [cond-mat.soft].
[2] E. Schneider and H. Stark, arXiv:1909.03243v1 [cond-mat.soft].

A mesoscale model for liquid-vapor phase transition over solid surfaces

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A novel continuum diffuse interface model en- dowed with thermal fluctuations [1] will be extend- ed to address nucleation over surfaces and the successive hydrodynamic interactions of the bubbles among themselves and with the wall [2,3]. The potential impact of the model stems from a combination of sound physical modeling and computational effectiveness that, combined, allow to deal with realistic systems on macrosco- pic time intervals, from the microscopic nucleation phase to the later stages at hydrodynamic scales. To substantiate the claim, basic elements of the back-ground theory will be presented and seve- ral numerical simulations of bubble nuclea-tion/ dynamics will be discussed to demonstrate model strength and weaknesses in dealing with wettabi- lity-dependent phase transitions.

[1] M. Gallo, F. Magaletti, C.M. Casciola, Physical Review Fluids, 3, 053604 (2018).
[2] F. Magaletti, L. Marino, and C.M. Casciola, Phy- sical Review Letters 114, 064501 (2015).
[3] F. Magaletti, M. Gallo, L. Marino, and C. M. Casciola, International Journal of Multiphase Flow, 84, 34 (2016).

Fluid-mediated interactions between colloids in bulk and confinement

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The behavior of colloids can be effectively controlled by tuning the solvent-mediated interactions among them. In this contribution, we shall briefly describe the physics of such colloid-colloid interactions in bulk systems [1] and how the interactions are modified in the presence of a surface and in confinement. One finds strong non-additivity of solvent-mediated interactions and significant effects of confinement on the colloidal phase behavior [2]. We shall also discuss the confinement-induced formation of capillary bridges between the colloids as well as the accompanying bridging phase transitions. In addition, we shall describe interface localization-delocalization transitions, which may occur in two-phase fluids confined to a slit, and how colloids facilitate its detection [3].

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[1] A. Maciołek and S. Dietrich, Collective behavior of colloids due to critical Casimir interactions, Rev. Mod. Phys. **90**, 045001 (2018).

[2] O. A. Vasilyev, S. Dietrich, and S. Kondrat, Nonadditive interactions and phase transitions in strongly confined colloidal systems, Soft Matter **14**, 586 (2018).

[3] S. Kondrat, O. A. Vasilyev, and S. Dietrich, Probing interface localization–delocalization transitions by colloids, J. Phys.: Condens. Matter **30**, 414002 (2018).

Instabilities of Liquid Crystal Films on Nanoscale

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This contribution focuses on recently developed models and computational techniques for thin films, with focus on nematic liquid crystal films. Models and computations are developed within the framework of long wave approach, augmented by inclusion of liquid-solid interaction forces via disjoining pressure model. Particular aspect that will be discussed includes inclusion of liquid-crystalline nature of the film in the model in a tractable manner. The simulation techniques include algorithms for GPU computing that allow for simulations of large domains and analysis of various instability mechanisms. Further details about implementing modeling techniques and GPU computing methods can be found in [1, 2].

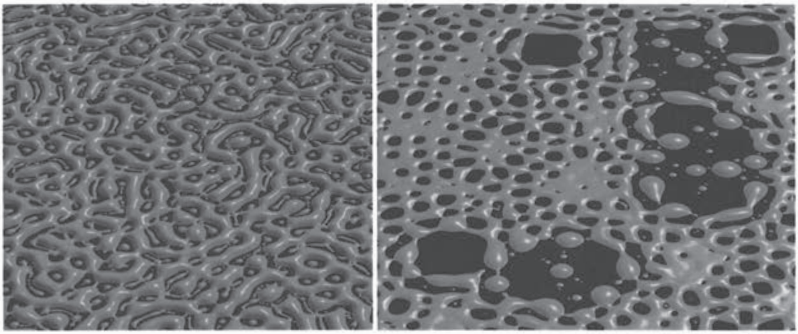

FIG. 1. Examples of liquid crystal film instabilities: (left) subject to random infinitesimal perturbations, and (right) subject to a mixture of random and localized perturbations (acting as nucleation centers). From [2].

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[1] M. Lam, L. Cummings and L. Kondic, J. Fluid Mech. **841**, 925 (2018)
[2] M. Lam, L. Cummings and L. Kondic, J. Comp. Phys. X **2**, 100001 (2019)

Large-scale molecular dynamics simulations of inhomogeneous fluids: the boundary matters

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Fluids exhibit a plethora of phenomena at macroscopic scales, which have their origin in the interactions between molecules. Often pair interactions are sufficient to generate interesting behaviour such as phase coexistence, adsorption films, and critical dynamics. We have used massively parallel, large-scale molecular dynamics simulations to investigate these phenomena at the molecular scale and to test predictions from statistical mechanics and continuum theories. In each case, the role of the type of boundary is highlighted.

Scattering techniques are a main probe of fluids at the molecular scale, however, the signal from an interface is typically buried by fluctuations of the adjacent bulk phase(s). For planar liquid-vapour interfaces, we have simulated scattered intensities, which are in remarkable agreement with recent predictions from density functional theory. An effective, scale-dependent surface tension with a strictly positive bending coefficient is obtained by isolating the interfacial structure factor relative to a reference state of coexisting homogeneous fluids.

As a by-product upon constructing this reference, we note that the compressibility of a liquid slab, confined by open boundaries, shows significant deviations of either sign from its bulk value. Open boundaries apply also if subvolumes of a large simulation box are considered. Here, a finite-size scaling analysis of a binary fluid close to its consolute point shows that the critical Binder cumulant is markedly different for open and periodic boundary conditions.

Confining binary fluids to a planar slit pore imposes impenetrable boundaries. Upon quenching the fluid from the mixed, homogeneous phase to its consolute point, critical fluctuations develop and an adsorption film builds up. Using non-equilibrium molecular dynamics simulations, we study the dynamic response and the equilibrium adsorption profiles, both exhibit scaling compatible with the universality class of model *H'*. For narrow confinement, critical Casimir forces develop between the two walls, which gives insight into the dynamics of this effective interaction. Our simulation results reveal a rich structure of correlation functions including slow, algebraic decays.

Non-equilibrium interfaces of patchy colloids in 2 and 3D

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We investigate the self-organization of patchy colloidal particles deposited on flat substrates in three (2+1) and two (1+1) spatial dimensions. We propose and use a simple stochastic model for the interaction between the particles, which allows the simulation of very large systems, to probe the long time and large-scale structure of the deposited films. The latter exhibit well defined surface, liquid and interfacial regions except when the growth is dominated by the formation of chains, which occurs for systems with an effective valence close to two. We consider both diffusive and ballistic deposition. For ballistic deposition we investigate the interfacial roughening in (1+1) systems and compare our results with those obtained experimentally for colloidal deposits left by evaporating droplets. We find, in line with the experiments, that when the film growth is dominated by chains the generic Kardar-Parisi-Zhang (KPZ) interfacial roughening is replaced by quenched KPZ. We discuss this somewhat surprising result.

References

1. "Nonequilibrium growth of patchy-colloid networks on substrates", C. S. Dias, N. A. M. Araújo and M. M. Telo da Gama, Physical Review E **87**, 032308 (2013).
2. "Nonequilibrium adsorption of 2AnB patchy colloids on substrates", C. S. Dias, N. A. M. Araújo and M. M. Telo da Gama, Soft Matter **9**, 5616 (2013).
3. "Mixtures of functionalized colloids on substrates", C. S. Dias, N. A. M. Araújo and M. M. Telo da Gama, Journal of Chemical Physics **139**, 154903 (2013).
4. "Kinetic roughening of aggregates of patchy colloids with strong and weak bonds", C. S. Dias, N. A. M. Araújo, and M. M. Telo da Gama, Europhysics Letters **107**, 56002 (2014).
5. "Adsorbed films of three-patch colloids: Continuous and discontinuous transitions between thick and thin films", C. S. Dias, N. A. M. Araújo, and M. M. Telo da Gama. Physical Review E **90**, 032302 (2014).
6. "Kinetic interfaces of patchy particles", N. A. M. Araújo, C. S. Dias and M. M. Telo da Gama, Journal of Physics: Condensed Matter **27**, 194123 (2015).
7. "Nonequilibrium self-organization of colloidal particles on substrates: adsorption, relaxation, and annealing", N. A. M. Araújo, C. S. Dias, M. M. Telo da Gama, Journal of Physics: Condensed Matter 29 (1), 014001 (2017).
8. "Dynamics of Network Fluids", C. S. Dias, N. A. M. Araujo, M. M. Telo da Gama, Advances in Colloids and Interface Science **247**, 258 (2017).
9. "Annealing cycles and the self-organization of functionalized colloids", C. S. Dias, N. A. M. Araujo, M. M. Telo da Gama, Journal of Physics: Condensed Matter **30** 014001 (2018).
10. "Shape anisotropy and the aggregation of colloidal particles at the edge of an evaporating drop", C. S. Dias, P. J. Yunker, A. G. Yodh, N. A. M. Araújo and M. M. Telo da Gama, Soft Matter **14**, 1903-1907 (2018).

Wetting of Yield-Stress Fluids

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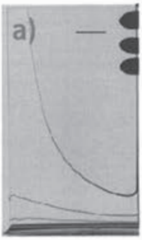
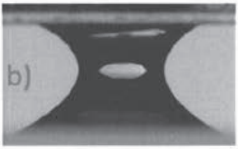
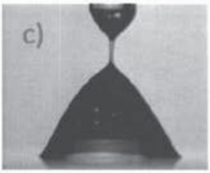
Yield-stress fluids such as foams, gels, emulsions exhibit an intermediate behaviour between elastic solids and viscous liquids. Indeed, when these materials are submitted to low stresses, they deform elastically and beyond a so-called "yield" stress, they flow like liquids. This intermediate solid/liquid behaviour is very useful for many applications, so that these complex fluids are omnipresent in food processing, cosmetics, construction, etc. However, from a more fundamental point of view, this intermediate liquid/solid behaviour makes their description and understanding more difficult. In this presentation, I will focus on the wetting properties of yield-stress fluids, namely I will study how they spread, how they interact with walls or capillaries and which shape they adopt. Whereas the wetting of simple Newtonian fluids is an old problem, the wetting of yield-stress fluids has generated a great deal of interest in the last ten years [1-5]. Through three classical wetting experiments - capillary ascension a), capillary bridge b) and drop spreading c) - carried out with dense suspensions of polymer microgels, I will show the importance of the competition between the yield-stress and the surface tension [6,7] and more surprisingly I will show the importance of the boundary conditions [6,8] and the flow history [7]. Finally I will show that the adopted shape or the height reached during capillary rise correspond to a dynamical arrest instead of a thermodynamical equilibrium [6].







References

[1] J. Boujlel et al. Soft Matter **9**, 5898 (2013).
[2] M. Maillard et al. Physical review letters **112**, 068304 (2014).
[3] G. German et al. J. Phys Cond Matt **21**,375111 (2009).
[4] G. German et al. Physics of fluids **22**, 033101 (2010).
[5] W. Smit et al. (2019).
[6] B. Géraud et al. Europhysics Letters **40**, 5 (2014)
[7] L. Jørgensen et al. Soft Matter **11**, 5111 (2015)
[8] J. Péméja, et al. Phys Rev Fluids **4**, 033301 (2019)

Taming bacterial turbulence by external fields and arrays of obstacles

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Active systems spontaneously self-organize into complex spatio-temporal structures such as flocks, bands, and vortices. These collective states are susceptible to constraints, e.g., geometrical confinement or orienting external fields. Here, we investigate the impact of such constraints on mesoscale turbulence, a state emerging in bacterial suspensions which is characterized by the chaotic dynamics of vortices with a characteristic size [1]. To this end, we apply a recently derived fourth-order field theory for a vectorial order parameter representing an effective microswimmer velocity [1].

First, we show how the application of an orienting external field (representing processes like magneto-, gravi-, chemo- or phototaxis) suppresses the turbulent state and stabilizes a traveling stripe pattern [2]. Second, by a combination of continuum theory [1] and experiment on a suspension of motile bacteria *Bacillus Subtilis* [3], we unravel the role of self-induced topological defects imposed by tiny obstacles (pillars) on the local flow profile of the active fluid. This approach enables the design of bacterial vortex lattices with tunable local order. Beyond the stabilization of square [3] and hexagonal lattices, we provide a striking example of a chiral, antiferromagnetic lattice induced by arranging obstacles in a Kagome-like array [4]. Here, the interplay of the lattice topology and bacterial activity generates a net rotational flow, hinting at novel ways for microcargo transport.

References

[1] H. Reinken, S. H. L. Klapp, M. Bär, and S. Heidenreich, Phys. Rev. E, **97,** 022613 (2018)
[2] H. Reinken, S. Heidenreich, M. Bär, and S. H. L. Klapp, New. J. Phys., **21**, 013037 (2019)
[3] D. Nishiguchi, I. S. Aranson, Alexey Snezhko, and Andrey Sokolov, Nat. Comm. **9**, 4486 (2018)
[4] H. Reinken, S. Heidenreich, D. Nishiguchi, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, to be submitted

Active colloids swimming at oil-water interfaces

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A common way to achieve propulsion at the colloidal scale is to produce artificial particles that have asymmetric shapes and surface properties. I will describe recent work in our group where we take well-known micro-swimmers that are propelled by self-generated asymmetrical chemical gradients (Janus swimmers) and we confine their motion at an oil-water interface. Two-dimensional confinement and interactions with the fluid interface strongly affect the propulsion speed and the directionality of the particle trajectories [1]. Furthermore, we study how the swimmers interact with complex environments constituted by self-assembled arrays of passive obstacles. Here, we find that two orientations of the active colloids exist, which lead to different coupling with lattices of passive particles [2]. Fast particles (active interstitials), which interact weakly with the obstacles, effectively only change their orientation through collisions. Slower particles, which are strongly coupled to the lattice of passive obstacles (active atoms), instead exhibit intermittent motion and contribute to structural rearrangements of the surrounding monolayers. I will finish by showing preliminary results where swimming is introduced by localized surface tension gradients stemming from asymmetric heating and show the potential for the realization of active monolayers of colloids trapped at a fluid interface.

References

[1] K Dietrich, D Renggli, M Zanini, G Volpe, I Buttinoni and L Isa, New Journal of Physics, **19**, 065008 (2017)

[2] K Dietrich, I Buttinoni, G Volpe and L Isa, Phys. Rev. Lett. **120**, 268004 (2018)

Microgels at liquid-liquid interfaces

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Microgels are soft particles individually made by cross-linked polymer networks which are nowadays widely used as a colloidal model system because of their swelling properties and their responsivity to external control parameters such temperature or pH. While extensively used as model systems in experimental, their numerical investigation lagged behind due to the inherently complex and multiscale nature of the particles. To this aim, we recently developed a numerical protocol to synthesize realistic microgels in-silico. In this contribution I will discuss the extension of this framework to investigate microgels at liquid-liquid interfaces in comparison with experimental results [1]. Next, I will report the calculation of elastic properties and effective interactions at the interface [2] comparing with available theoretical models. Our work aims to establish a clear link between the microscopic properties and the resulting microgel-microgel interactions, paving the way for a deeper understanding of the collective behaviour of microgel suspensions.

References

[1] F. Camerin, M.A. Fernandez-Rodriguez, L. Rovigatti, M.-N. Antonopoulou, N. Gnan, L. Isa and E. Zaccarelli, ACS Nano 13, 4548 (2019).
[2] F. Camerin, N. Gnan, J. Ruiz-Franco, A. Ninarello, L. Rovigatti and E. Zaccarelli, submitted (2019).

Droplets dynamics from wall texturing to liquid surfaces

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Manipulation of multiphase liquids is pivotal in microfluidics, either we focus on complex flows in closed microchannels or sessile drops moving on open surfaces.
Albeit the fluidization of soft-glassy materials (SGMs) is strongly affected by the surface texturing, the effect of the geometry has not been addressed so far [1, 2]. We describe how the fluidization of jammed emulsions can be controlled by wall roughness textured by microgrooves. We report a scaling law for the roughness-induced fluidization as a function of the grooves' density and the existence of two fluidization scenarios belong to different grooves' separation [3,4]. By introducing a herringbone texturing of the grooves, the flow along converging herringbones results faster with respect to the diverging geometry, even below the jamming point. This asymmetry is not simply triggered by herringbone mixing. In open microfluidics, we report the one-dimensional motion of few microliters drops of liquids with different viscosities and surface tensions on inclined plate subject to vertical sinusoidal oscillation with frequency ranging from tens up to hundreds of Hz. We have taken into account both surfaces with finite contact angle hysteresis and Lubricate-Infused Surfaces (LIS), characterized by low hysteresis [5]. The main difference between the two substrates is the presence of drop pinning for the former, and the switch between sliding down and climbing up for the latter.

References

[1] V. Mansard *et al*. Soft Matter **10**, 6984-6989 (2014)
[2] J. Goyon *et al.*, Nature **454**, 84-87 (2008)
[3] L. Derzsi *et al.*, Phys. Rev. E **95**, 052602 (2016)
[4] L. Derzsi *et al.*, Soft Matter **14**, 1088-1093 (2018)
[5] P. Sartori et al. J. Fluid Mech, **882**, R4 (2019)

Active particles near substrates: from biofilms to colloids in motility patterns

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Self-propelled "active" particles typically aggregate on two-dimensional planar substrates performing quasi two-dimensional motion. Here we discuss recent results for active particles near such substrates. First of all we propose a simple model for biofilms exploring the hydrodynamic flow towards the film as induced by the self-propulsion of the particles in the film [1]. Second we consider active colloids in various motility patterns [2] and discuss a colloidal brazil nut effect [3] as well as motility-induced flashing [4] and trapping.

References

[1] A. J. T. M. Mathijssen, F. Guzman-Lastra, A. Kaiser, H. Löwen, Physical Review Letters **121**, 248101 (2018)

[2] C. Lozano, B. ten Hagen, H. Löwen, C. Bechinger, Nature Communications **7**, 12828 (2016)

[3] S. Jahanshahi, B. ten Hagen, C. Lozano, C. Bechinger, H. Löwen, J. Chem. Phys. **150**, 114902 (2019)

[4] C. Lozano, B. Liebchen, B. ten Hagen, C. Bechinger, H. Löwen, Soft Matter **15**, 5185 (2019)

Droplets of complex fluids on walls

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We present quantitative contact angle measurements of droplets from a phase separated colloid-polymer mixture on walls coated with different polymers. The colloid-polymer system consists of an aqueous suspension of poly(methyl methacrylate) particles and xanthan polymer, whereas the walls are coated with either polyacrylamide or chitosan. By fitting the shape of the droplet taking gravity and surface tension into account the contact angle can be determined, even when the radius of the drop is only an order of magnitude larger than the surface roughness. The setup further allows studying strongly confined interfaces between walls with different wetting conditions. Finally, the applicability of the approach is illustrated for biological systems.

Challenges of modelling the moving contact line problem and recent progress: bridging scales from the nano- to the macroscale

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The moving contact line problem occurs when modelling one fluid replacing another as it moves along a solid surface. Classically, the no-slip boundary condition at the solid substrate and motion at the three-phase contact line are incompatible - leading to the well-known shear-stress singularity [1]. Here we will review progress made by our group considering the moving contact line problem and related physics from the nano- to macroscopic lengthscales. Specifically, to capture nanoscale properties very close to the contact line and to establish a link to the macroscale behavior, we employ elements from the statistical mechanics of classical fluids, namely density-functional theory (DFT). We formulate a new and general dynamic DFT (DDFT) that carefully and systematically accounts for the fundamental elements of any classical fluid. In a certain limit, our DDFT reduces to a non-local Navier-Stokes-like equation [2]. Work analyzing the contact line in both equilibrium and dynamics will be presented [3,4]. The new model allows us to benchmark existing phenomenological models and reproduce some of their key ingredients. But its multiscale nature also allows us to unravel the underlying physics of moving contact lines, not possible with any of the previous approaches, and indeed show that the physics is much more intricate than the previous models suggest.

References

[1] D.N. Sibley, A. Nold and S. Kalliadasis, J. Fluid Mech. **764**, 445 (2015)
[2] B.D. Goddard, A. Nold, N. Savva, P. Yatsyshin and S. Kalliadasis, J. Phys.: Condens. Matter **25**, 035101 (2013)
[3] A. Nold, D.N. Sibley, B.D. Goddard and S. Kalliadasis, Phys. Fluids **26**, 072001 (2014)
[4] A. Nold, PhD Thesis, Imperial College (2016)

Experimental observation of flow fields around active Janus spheres

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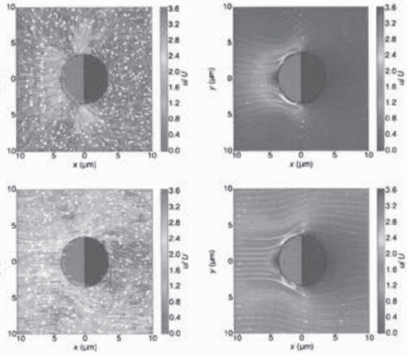
The phoretic mechanisms at stake in the propulsion of asymmetric colloids have been the subject of debates during the past years. In particular, the importance of electrokinetic effects on the motility of Pt-PS Janus sphere was recently discussed. Here, we probe the hydrodynamic flow field around a catalytically active colloid using particle tracking velocimetry both in the freely swimming state and when kept stationary with an external force. Our measurements provide information about the fluid velocity in the vicinity of the surface of the colloid, and confirm a mechanism for propulsion that was proposed recently. In addition to offering a unified understanding of the nonequilibrium interfacial transport processes at stake, our results open the way to a thorough description of the hydrodynamic interactions between such active particles and understanding their collective dynamics.



Reference

A. I. Campbell, S. E. Ebbens, P. Illien, R. Golestanian, Nat. Comm. **10**, 3952 (2019)

Abstracts of Posters

(in alphabetical order)

Pore-scale direct numerical simulation of Haines jumps in a porous media model

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We present direct numerical simulations for a porous media model consisting of two immiscible fluids in a micro-geometry filled with randomly sized and randomly distributed cylinders. First, interface instability and penetration modes are presented when varying the wetting features of the porous medium, showing that the displacement patterns not only change with the capillary number, but also are a function of the contact angle, even for a viscosity ratio of unity. This is an important conclusion suggesting that capillary number and viscosity ratio alone cannot completely describe the pore-scale displacement. Second, rapid pore-scale displacement is considered, where the displacements are accompanied by sudden interface jumps from one site to another, known as Haines jumps. The characteristic time and length scales of a Haines jump are examined. This work is in collaboration with Adam O'Brien and Markus Bussmann from the University of Toronto.

Surface Wetting to Cleaning-In-Place Optimisation

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During product manufacturing, deposits adhere to industrial surfaces forming layers that are difficult to remove - about 80% of the total production costs could be attributed to fouling and cleaning.[1] Some of the current challenges for researchers is to reduce fouling and cleaning costs by optimisation of Clean-In-Place technique. Some surface parameters such as composition, roughness, and temperature can affect fouling induction, build-up and removal, however, the involved interactions in a real food-contact environment require further investigation. The aim of this research is to obtain a better comprehension of the impact that the main surface variables (e.g. topography, temperature, and surface free energy), before and after foulant deposition, have on fouling development during product manufacturing. The objectives are (i) to study wettability of cleaned and fouled stainless steel surfaces, and (ii) to quantify surface free energy of both substrates as a function of temperature. Foulant model is formed by a Whey Protein solution.

Total surface free energy of cleaned stainless steel does not change notably as a function of temperature (20-80°C). However, it is increased for rougher substrates ($Ra < 0.83$ µm; standardised roughness limit for food-contact surfaces[2]). Upon foulant deposition, there was an increased system hydrophobicity. Non-polar liquids seem to be not dissolved on the WP layer. This greater hydrophobicity and no reaction with non-polar liquids could help to understand fouling build-up as well as the later cleaning performance. Total SFE of deposits also remains constant as a function of temperature. However, there was an increase of foulant polarity around 3.38%, from 25 to 80°C. Increased polarity by temperature could also play an important role on the interactions between food-polar compounds and the deposited material. For instance, milk proteins and minerals could be more attracted to the top of the initial fouling layer, developing a more compacted fouling structure - Ca^{2+} promotes protein aggregation forming bridges between adsorbed protein and bulk proteins.[3,4] The results so far demonstrate that the temperature difference between liquid and substrate, surface finish and its composition, liquid properties, as well as characteristics of the deposited foulant are competing for the control of the complex fouling phenomena, and consequently, the efficiency of CIP systems.

References

[1] Van Asselt et al., Food & Bioproducts Processing **80**, 276–280 (2005).
[2] Frantsen and Mathiesen, NACE corrosion, paper 09573 (2009).
[3] Xiong, Journal of Agricultural and Food Chemistry **40**, 380–384 (1992).
[4] Pappas and Rothwell, Food Chemistry **42**, 183-201 (1991).

Charge-driven interfacial gelation of cellulose nanofibrils across the water/oil interface

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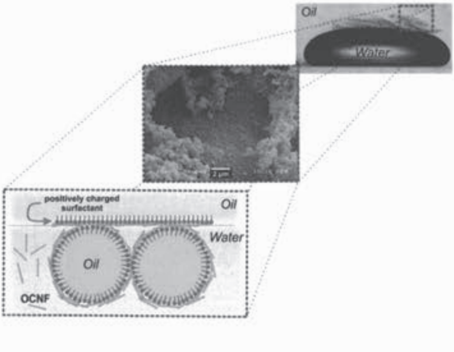
Understanding the assembly of cellulose nanoparticles at water/oil (W/O) interfaces, underpins the use of these easily prepared biobased particles in formulated products. In this study we investigate the spontaneous adsorption of oxidised cellulose nanofibrils (OCNF) across planar W/O interfaces under conditions where bulk contributions are negligible, allowing exploration of the interfacial phenomena alone. Spontaneous adsorption of the water-dispersible OCNF across the W/O interface was induced by employing an oppositely-charged oil-soluble surfactant. This approach relies on the use of two immiscible liquids as scaffolds, delivering two oppositely- charged species and directing a charge-driven complexation across the W/O interface. Interfacial rheology experiments showed that, upon complexation of OCNF and the oppositely charged surfactant, interfacial gels were produced, and different interfacial properties obtained by modulating the ζ-potential of the OCNF (by electrolyte addition). Spontaneous OCNF adsorption at the W/O interface occurred for particles with ζ-potential more negative than -30 mV, resulting in the formation of interfacial gels; whilst for particles with ζ-potential of *ca.* -30 mV, spontaneous adsorption occurred coupled with augmented interfibrillar interactions, yielding stronger and tougher interfacial gels. Contrarily, charge neutralisation of OCNF (ζ-potential values more positive than -30 mV) did not allow spontaneous adsorption of OCNF at the W/O interface. In the case of favourable OCNF adsorption, the interfacial gel was found to embed oil-rich droplets - a spontaneous emulsification process (Figure 1). The development of interfacial gels has implications for capsule formation and tuning in O/W emulsions – systems where interfacial rheology studies are extremely challenging, yet where tuneability is key to utility.



Propagation of interfaces in active liquid crystals on a substrate

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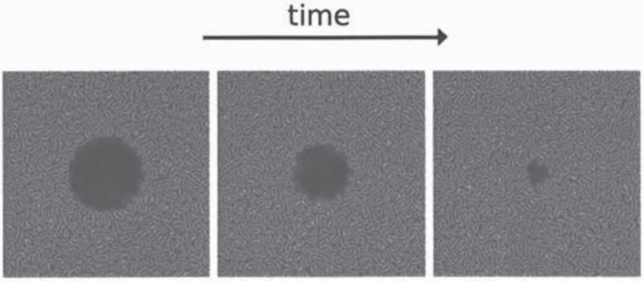
In Nature, there are systems formed by many elongated units or particles capable of transforming the energy of the environment in directed motion. Examples are dense suspensions of bacteria, mixtures of microtubule-kinesin and shoals of fish. These systems exhibit collective dynamics that in many cases may be described by the hydrodynamic equations of active liquid crystals. As in passive liquid crystals, active ones may be in the nematic phase (where particles align along a preferred direction) or in the isotropic one (disordered) in addition to complex dynamical phases at high activities. In this poster, we present results of numerical simulations of the propagation of isotropic-nematic interfaces of active liquid crystals on a substrate. We analyze how the dynamics of the interface changes with the activity and with the friction with the substrate. We find that the correlation function of the velocity scales with the activity length. In addition, the energy spectrum of the active nematic and the structure factor of the interface follow (approximately) the same power laws as those reported for bacterial swarms of *Serratia marcescens*.



References

[1] R. C. V. Coelho, N. A. M. Araújo and M. M. Telo da Gama, Soft Matter, **15**, 6819-6829 (2019)

[2] A. E. Patteson, A. Gopinath & P. E. Arratia, Nature Communications, **9**, 5373 (2018)

From cellular to tissue mechanics: Fluidization based on topological activity

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Vertex models similar to those initially introduced to describe liquid-air foams have been applied to the study of epithelial tissues. Cells are represented as polygons, and tri-cellular junctions are represented as edges (called vertices). Up to now, those models have essentially been used to infer the final shape formation, which is supposed to correspond to a minimal energy state.

Here, we propose a dynamics for the vertices that is based on active gel theory, which is a hydrodynamic description of the actin-myosin complex - hence including an active stress term to account for the contractile forces generated by molecular motors. This dynamical vertex model enables us to address question relative to tissue-scale fluctuations (e.g. dossal closure) or to the time scale required for organ formation.

In our models, we include topological changes such as cell division, cell death, and neighbor exchange. These changes fluidize tissues thereby facilitating large scale morphological changes.

Furthermore, to incorporate curvature effects during organogenesis, we developed three dimensional models using computer simulations.

References

[1] Priti, A., Ong, H.T., Toyama, Y., Padmanabhan, A., Dasgupta, S., Krajnc, M. and Zaidel-Bar, R., 2018. Syncytial germline architecture is actively maintained by contraction of an internal actomyosin corset. *Nature communications*, *9*(1), p.4694.

[2] Krajnc, M., Dasgupta, S., Ziherl, P. and Prost, J., 2018. Fluidization of epithelial sheets by active cell rearrangements. *Physical Review E*, *98*(2), p.022409.

[3] Dasgupta, S., Gupta, K., Zhang, Y., Viasnoff, V. and Prost, J., 2018. Physics of lumen growth. *Proceedings of the National Academy of Sciences*, *115*(21), pp.E4751-E4757.

Condensation frosting on nanostructured surfaces

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Anti-icing surfaces are of great interest in areas such as aeronautics, energy transport, infrastructure and refrigeration. Several experiments in dry atmosphere have shown that micro and nanostructured superhydrophobic surfaces, cooled to below zero temperature, can delay the freezing of sessile drops compared to a flat hydrophobic surface. This is due to a smaller solid-liquid interface that reduces the probability of heterogeneous ice nucleation and the latent heat flow. However, they may fail in a humid real environment because water vapour undergoes condensation frosting. Condensate embryos nucleate between the micro and nanostructures; if the condensate droplets are energetically favoured to grow in a Wenzel state, they will cause the loss of the superhydrophobic state of a sessile drop. Indeed, the amount of air trapped under the sessile drop will decrease as the coalescence with the penetrated condensate goes on. Therefore, in addition to the loss of superhydrophobicity, the result is that both the condensate droplets and the sessile drop freeze quickly due to a high solid-liquid interface. A key aspect to consider when designing an anti-icing surface is how the morphology of the surface can direct the condensate growth. As shown in recent studies, slender, tapered and densely packed nanostructures permit the condensate growth towards the apex of the structures in a partially suspended Cassie state that favours the droplets jumping induced by coalescence. In the case of a surface cooled under 0 °C, a condensate droplet in the Cassie state freezes later than one in the Wenzel state, which globally leads to a delay of the condensation frosting phenomenon. In the present experimental study, silicon surfaces with random nanostructures have been realized by combining metal dewetting and metal assisted chemical etching (MacE). Nanopillars and nanocones with different tapering have been obtained varying the composition of the etching solution and made hydrophobic with an FDTS coating. The experiments has been conducted placing the surfaces on a cold plate in a chamber with controlled humidity. Optical microscope observations have permitted to evaluate the condensation path and the condensation frosting dynamic at different plate temperatures and chamber humidity.

Theoretical study of liquid metal wetting

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The wetting properties of liquid metals on diamond surfaces is strongly dependent on the roughness of the diamond surface. As shown by Escobar et al., super-phobic surfaces can be achieved with roughness to the degree that the liquid metal drop behaves as a solid with almost zero wetting. Furthermore, mercury has an unusual dielectric function at low frequencies, is not described by a typical Drude model but by an approximation known as the Drude-Smith model. The role in the retarded van der Waals /Casimir forces between liquid metals and Au was calculated in previous works (2).

In this work, we make a theoretical study of the wetting of liquid metals and diamond surfaces.
The dielectric function. We consider mercury and eutectics InGa at room temperature. Using the Lifshitz theory of dispersive interactions, we calculate the adhesion force between the mercury and the diamond as well as the contact angle. To take into account the dielectric function of the rough diamond surface, we use an effective medium approximation assuming random roughness.
Finally, we consider other materials other than diamond surfaces that will yield super phobic behavior.

References

(1) J. V. Escobar and R. Castillo, Force of adhesion upon loss of contact angle hysteresis: when a liquid behaves like a solid, Phys. Rev. Lett. 111, 226102, (2013).
(2) R. Esquivel-Sirvent and J. V. Escobar, Casimir force between liquid metals, Europhys. Lett. 107, 40004, (2014).

Tricritical Casimir forces and order parameter profiles in wetting films of ^{3}He – ^{4}He mixtures

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Tricritical Casimir forces in ^{3}He – ^{4}He wetting films are studied [1], within mean field theory, in terms of a suitable lattice gas model for binary liquid mixtures with short–ranged surface fields. The proposed model takes into account the continuous rotational symmetry O(2) of the superfluid degrees of freedom associated with ^{4}He and it allows, inter alia, for the occurrence of a vapor phase. As a result, the model facilitates the formation of wetting films, which provides a strengthened theoretical framework to describe available experimental data [2] for tricritical Casimir forces acting in ^{3}He – ^{4}He wetting films.

References

[1] N. Farahmand Bafi, A. Maciołek, and S. Dietrich, Phys. Rev. E **95**, 032802 (2017).
[2] R. Garcia and M. H. W. Chan, Phys. Rev. Lett. **88**, 086101 (2002).

Tuning the geometry of bioinspired biphilic surfaces for efficient water collection and transport

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The Namib desert beetle has developed a water collection mechanism based on biphilic surfaces: hydrophilic patches are embedded in a hydrophobic wax layer, improving water nucleation, droplet growth and transport of water into the mouth of the beetle.[1] Synthetic surfaces successfully collect water from humid air.[2] To improve collection efficiency water condensation and droplet transport, surface properties can be tuned, such as patch size, geometry and area fraction of the patches. A critical part involves a fast droplet removal to free space for further water nucleation. Design drawbacks include a large contact angle hysteresis due to droplet pinning.

In this work, droplet nucleation, growth, and roll-off are studied on asymmetric patches. The morphology of water droplets on biphilic surfaces is compared to finite element simulations (Surface Evolver). The surfaces are prepared by spray coating of gold nanoparticles on hydrophobic substrates through a mask (Fig 1b). This geometric patch tuning enforces droplet coalescence on hydrophilic patches to form droplets of different shapes shown by FEM simulations (Fig. 1a). Droplet nucleation and coalescence on these surfaces are analyzed in a custom made environmental chamber with temperature and humidity ranges between 5 °C to 50 °C and 10% RH to 85% RH, respectively. The effect of patch asymmetry on pinning is analyzed by monitoring droplet roll-off angles and speeds depending on shape direction. To minimize droplet pinning, a size gradient is imposed from 500 μm down to 60 μm for a l/w ratio of 1 (Fig 1c). Intelligent design of biphilic surfaces can improve droplet formation and coalescence on them and therefore the efficiency of water collection.

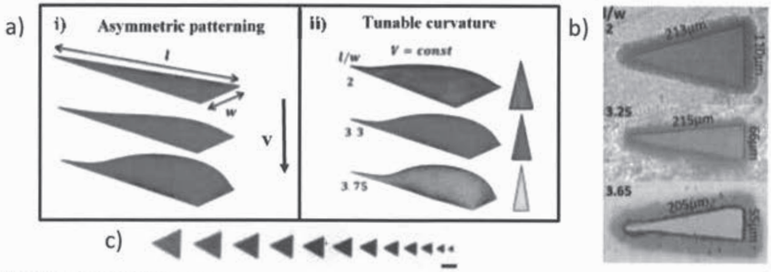

Figure 1 Droplet configuration on a chemically patterned hydrophilic wedge using finite element analysis (Surface evolver). a.i) A droplet with increasing volume on a wedge with l/w = 3.3. Volume (V^*) is scaled to the capillary length (l_c= 2.7 mm for water). ii)droplet shape at varying l/w = 2 (top), 3.3 (middle) and 3.75 (bottom). b) Pictures of masks for preparation of biphilic patterns. c) Microscope images of a size gradient of a biphilic surface with hydrophilic patches (copper; scale bar = 100μm)

[1] Parker, A. R.; Lawrence, C. R. Water Capture by a Desert Beetle. *Nature* **2001**, *414*, 33.
[2] Pinchasik, B.-E.; Kappl, M.; Butt, H.-J. Small Structures, Big Droplets: The Role of Nanoscience in Fog Harvesting. ACS Nano 2016, 10 (12), 10627–10630.

Nonequilibrium dynamics of the critical Casimir force

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The critical Casimir force (CCF) has so far been primarily discussed under equilibrium conditions. Here, the CCF is investigated as a function of time in a non-equilibrium situation [1,2]. Specifically, a temperature quench of a Landau-Ginzburg model with conservative dynamics (model B) is considered, focusing on a film geometry under symmetry-breaking as well as non-symmetry-breaking boundary conditions. The relevance of the global and local conservation of the order parameter is discussed and the ensemble dependence of the CCF is highlighted.

References

[1] M. Gross, A. Gambassi, S. Dietrich, Phys. Rev. E **98**, 032103 (2018)
[2] M. Gross, C. M. Rohwer, S. Dietrich, Phys. Rev. E **100**, 012114 (2019)

A MC-optimized DFT for the Jagla fluid

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In classical Density Functional Theory (DFT) the mean-field (MF) approximation works well to describe the phase behavior of simple fluids like the square-well or Lennard-Jones fluid. However, when it comes to more complicated fluids like e.g. the Jagla fluid, characterized through a rather long ranged repulsive ramp and attractive well, mean-field DFT fails to predict the correct phase behavior and density profiles for low temperatures and high densities. Even a more elaborate perturbation DFT does not overcome this shortcoming. Hence, we present a DFT optimized through Monte Carlo (MC) data which, at the current state of this work, is capable of predicting in a good approximation the correct density profiles of the Jagla fluid in the test particle and slit geometries, even for high densities and low temperatures.

Drop Impact on Hot Plates: Contact, Rebound and the Formation of Holes

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Drops interacting with hot plates are interesting from applications, such as spray cooling, and fundamental points of view. If a drop slowly approaches a substrate heated above the so-called static Leidenfrost temperature, it will levitate on a layer of vapour, and no wetting occurs, whereas it simply wets the substrate below that critical temperature. The situation becomes much more complex for impacting drops, where the impact pressure and shear forces during spreading additionally act on the vapour layer, and the time scales of heat transfer between the substrates and the droplet become important. This results in a significantly higher dynamic Leidenfrost temperature.

Its value is hard to determine, even using sophisticated measurement techniques such as Total Internal Reflection imaging alone, as the scales of local contacts become very small and rapid. Even more interesting, complex wetting patterns far beyond "simple" nucleating, growing, and merging bubbles are observed in a broad temperature range using Ultra-fast Total Internal Reflection Imaging, which resolves the locations of wetted spots. Structures in the third dimension (local vapour layer heights) can be resolved by Ultra-Fast X-ray measurements at e.g. Argonne National Labs. The combination of both data yields a rich, unpreceded insight into the wetting and de-wetting dynamics. Those are employed to, e.g., (1) develop a new experimental criterion from simple top view imaging for the determination of the (static and dynamic) Leidenfrost point, (2) explain a relation of contact and rebound times on transparent and smooth metal substrates, and (3) revealing new correlations between 3D vapour layer dynamics and the locations of wetting.

Capillary instability of elastic solids

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Surface tension plays a key role for phenomena involving liquid interfaces. A prime example is the Rayleigh-Plateau instability, causing a liquid jet to break into droplets in order to minimise the surface energy. Remarkably, a similar capillary instability was observed in soft solids. Here we reveal the intricate morphologies that can be encountered during the capillary collapse of an elastic cylinder, from minimisation of capillary and elastic energy. Subsequently, we show the dynamical mechanism by which solutions are selected. It is found that near the onset of instability, the shapes resemble a "cylinders-on-a-string" configuration, while as the solid gets softer "beads-on-a-string" are observed. Our analysis explains recent experimental and numerical observations, and highlights how surface tension can dictate the mechanics of solids - provided that the solids are sufficiently soft.

Interfacial wetting of binary liquid mixtures near a colloid

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To understand the wetting phenomena of a colloid located at the liquid-vapor interface of binary liquid mixtures, we combine the interfacial wetting behaviors of three different planar interfaces: liquid-vapor, wall-liquid, and wall-vapor. These wetting behaviors are obtained within the sharp-kink approximation. The combination of the wetting behaviors under the same thermodynamic condition corresponds to the solution of the original problem. Depending on the mixing rules, we find two cases of solutions. (i) Under the exact mixing rule, we find three distinct wetting domains. (ii) Under the relaxed mixing rule, we find six different wetting domains. In addition, under the exact mixing rule, it is possible to make estimates for the contact angle.

Intracellular wetting regulates degradation of fluid compartments

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Phase separation generates functional, subcellular condensates with fluid-like properties. The mechanisms that degrade fluid phases in cells, however, are not fully understood. Clearance of condensates involves autophagy, a conserved pathway in which membrane sheets isolate portions of the cytosol to form autophagosomes, which then fuse with lysosomes for cargo breakdown. Here, we studied the assembly of autophagic membranes at fluid interfaces in both living and synthetic cells. A minimal physical model shows that interfacial tension determines whether isolation membranes will sequester the condensate entirely, or will prematurely close and degrade the condensate in a piece-meal fashion. In the latter case, curvature-inducing proteins confer a regulatory switch that associates isolation membranes with condensates, however, without degrading them. Our findings suggest that the autophagic breakdown of fluids is a wetting phenomenon, which is controlled by elasto-capillary feedback between the phase-separated condensate, the cytosol and the isolating membrane.

References (in revision)

Agudo-Canalejo, J.; Schultz, S.W.; Chino, H.; Saito, C.; Koyama-Honda, I.; May, A.I.; Brech, A.; Mizushima, N.; **Knorr, R. L.***; Wetting regulates autophagy of phase separated droplets and the cytosol.

Knorr, R. L.*; Franzmann, T.; Feeney, M.; Frigerio, L.; Dimova, R.; Hyman, A. A.; Lipowsky, R.; Mutual Remodelling of Biomolecular Condensates and Membranes.

Detachment work of prolate spheroids from fluid droplets

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Deformation of a spherical droplet or bubble containing a pair of prolate spheroidal particles on its surface is considered when equal but opposite forces are applied to the particles. The particles are placed opposite to each other, thus providing a symmetric problem that is more amenable to analytical treatment. The force-displacement curves, calculated as the particles are pulled apart, are found to be linear for small displacements. The deviation from the linear force–displacement behaviour occurs close to the point of detachment.

It is known that, in the absence of line tension, prolate and oblate spheroidal particles attach to fluid interfaces more strongly because they reduce the interfacial area more than spherical particles for a given particle volume (see e.g. [1]). However, the studies based on the free energy difference between a particle at the interface and in the bulk are not sufficient for determining the value of the detachment work. Our previous study of the case of spherical particles [2,3] demonstrated that the dissipated energy becomes an increasingly dominant component of the work done during the detachment of particles, as the particle to droplet size ratio decreases. This indicated the existence of a significantly higher energy barrier to desorption of very small particles, compared to the one suggested by their adsorption energy alone.

In the case of prolate spheroids, we investigate the effect of dissipation upon the minimum detachment work for different aspect ratios of the particles. We find that, even in the absence of line tension, it is easier to remove elongated particles from fluid interfaces than spheres because of lesser viscous dissipation of energy.

References

[1] G. B. Davies et al., J. Chem. Phys. **141**, 154902 (2014)
[2] R. Ettelaie and S. V. Lishchuk, Soft Matter **111**, 4251 (2015)
[3] S. V. Lishchuk and R. Ettelaie, Langmuir **32**, 13040 (2016)

Capillary adhesive contact between soft microparticles

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The Johnson-Kendall-Roberts (JKR) theory [1] has been well recognized to describe the adhesive contact between two deformable particles generated by adhesion energy competing with elasticity. We extend the JKR theory to investigate the adhesion in three-phase (liquid-solid-vapour) interactions.

To validate the theoretical extension, we characterize the capillary adhesion between two liquid-bridged agarose microparticles using a tailored nanomechanical tester. The new experimental setup allows to measure force-displacement *(F-d)* curves up to the resolutions of 10 nN and 10 nm for force and displacement, respectively, and simultaneously to acquire the images of contact area/profile between the two particles through an incorporated long-focal CCD microscope system (Fig. 1). We apply the JKR theory to fit the pull-off *F-d* curves measured during the separation of the two particles and consequently to determine adhesion energy $\Delta\gamma$ and particle elasticity E.

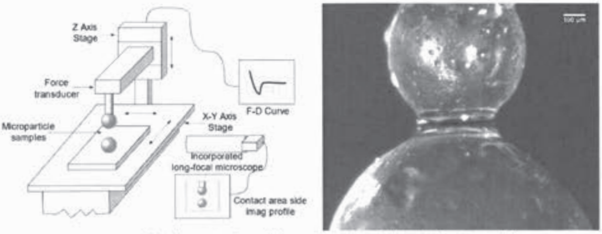

Fig. 1 (a) Schematic view of the nanomechanical tester (not to scale)
(b) The acquired image of the liquid bridge forming between two microparticles.

The results show the value of $\Delta\gamma$ (= 146±4 mN/m) is about twice the value of water surface tension γ_{LV}, while the value of E (= 79±2 kPa) is comparable to the agarose elasticity reported in the literature. A generalized Hertz theory proposed by Fogden and White [2] which adds the Laplace capillary condensation stress as the source of adhesive force demonstrates $\Delta\gamma=2\gamma_{LV}$ for two relatively soft and large objects in contact.

Our results confirm that JKR theory is valid for the capillary adhesion between two particles with a modified Tabor parameter [3] larger than 5 (i.e. soft and large particle contact).

References

[1] K.L. Johnson, et al., Proc. R. Soc. London A **324**, 301 (1971)
[2] A. Fogden, R.W. Lee, J. Colloid Interface Sci. **138**, 414 (1990)
[3] J. Sun, et al., Journal of Applied Mechanics **85**, 061009 (2018)

Wetting and dewetting of a nanoparticle at a polymer interface: numerical simulations based on a virtual work principle

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We present the results of numerical simulations showing the wetting and dewetting dynamics of a nanoparticle at a polymer interface. Our approach stems from a virtual work principle for calculating hydrodynamic flows in polymer blends in the presence of solid interfaces, and builds on the fluid particle dynamics method devised by Araki and Tanaka [1]. This approach enables us to solve coupled equations of motion for the polymer concentration field (Cahn-Hilliard) and the velocity field (Stokes), and to track the Gibbs free energy of the system as it relaxes towards equilibrium.

Simulations of a nanoparticle immobilised at the interface between two polymers show wetting timescales of the order of 10 µs. Dewetting simulations display the qualitative features predicted by theory, and observed experimentally, including the formation of a fluid rim in the early stages of dewetting. When shear is applied to the system, we may also observe the migration of the particle to its favoured polymer by a droplet-breaking mechanism. Quantitatively, the simulations show characteristic dewetting timescales of 1 to 100 µs, depending on the initial distance of the particle from the interface, and the shear rate applied to the system. They also indicate a critical film thickness (below which spinodal dewetting occurs) of the order of 5 nm, given the chosen range of the interactions. These results are consistent with other theoretical work and experimental observations.

References:

[1] T. Araki and H. Tanaka, *Physical Review E*, **73**, 061506 (2006)

Wettability and illumination-induced motion of Janus particle

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Using a fluid particle dynamics method we numerically investigate motion of a spherical Janus particle suspended in a binary liquid mixture, which emerge under heating of one-half of a colloid surface. The method treats simultaneously the flow of the solvent and the motion of the particle, hence, the velocity of the particle can be computed directly. Our approach accounts for a phenomenon of critical adsorption, therefore, a particle that is adsorptionwise nonneutral is always completely covered by an adsorption layer (droplet). In order to establish the mechanism of self-propulsion, we study systematically various combinations of adsorption preference on both hemi-spheres of the Janus colloid as function of the heating power for symmetric and nonsymmetric binary solvent and for various particle sizes in three spatial dimensions. Only for a particle, which heated hemisphere is neutral whereas the other hemisphere prefers one of the two components of the mixture, the reversal of the direction of motion occurs. The particle self-propels much faster in the nonsymmetric binary solvents. Self-propulsion originates from a gradient of mechanical stress, in a way similar to the Marangoni effect. This stress is not localized at the edge but distributed within the whole droplet. We compare our findings with the experimental observations and other theoretical results.

Electrostatic interaction of particles trapped at fluid interfaces: effects of geometry and wetting properties

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The electrostatic interaction between pairs of spherical or macroscopically long, parallel cylindrical colloids trapped at fluid interfaces is studied theoretically for the case of small inter-particle separations. Starting from the effective interaction between two planar walls [1] and by using the Derjaguin approximation, we address the issue of how the electrostatic interaction between such particles is influenced by their curvatures and by the wetting contact angle at their surfaces [2]. Regarding the influence of curvature, our findings suggest that the discrepancies between linear and nonlinear Poisson–Boltzmann theory, which have been noticed before for planar walls, also occur for spheres and macroscopically long, parallel cylinders, though their magnitude depends on the wetting contact angle. Concerning the influence of the wetting contact angle θ simple relations are obtained for equally sized particles which indicate that the inter-particle force varies significantly with θ only within an interval around 90°. This interval depends on the Debye length of the fluids and on the size of the particles but not on their shape. For unequally sized particles, a more complicated relation is obtained for the variation of the inter-particle force with the wetting contact angle.

References

[1] A. Majee, M. Bier, and S. Dietrich, J. Chem. Phys. **145**, 064707 (2016)

[2] A. Majee, M. Bier, and S. Dietrich, Soft Matter **14**, 9436 (2018)

Persistent correlations in colloidal suspensions

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Transport properties of a hard-sphere colloidal fluid are investigated by Brownian dynamics simulations. We implement a novel algorithm for the time-dependent velocity-autocorrelation function (VACF) essentially eliminating the noise of the bare random motion. The measured VACF reveals persistent anticorrelations manifested by a negative tail $t^{-5/2}$ at all densities [1]. At small packing fractions the simulations fully agree with the analytic low-density prediction, yet the amplitude of the tail becomes dramatically suppressed as the packing fraction is increased. The mode-coupling theory of the glass transition provides a qualitative explanation for the strong variation in terms of the static compressibility as well as the slowing down of the structural relaxation.

References

[1] S. Mandal, L. Schrack, H. Löwen, M. Sperl and T. Franosch accepted in **PRL** (in press) (2019).

Delayed dynamics of liquid droplet impact on multiscale super-hydrophobic surfaces

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The effect of surface friction on drop impact dynamics is investigated. When a drop of radius *R* impact a surface with a velocity *U*, it generally spreads and under certain conditions forms a lamella surrounded by a liquid rim. At intermediate Weber number, if the friction between the liquid and the surface is total, the spreading stops due to the development of a viscous boundary layer, after a time scale of $(U/R)\ \mathrm{Re}^{1/5}$ [1]. We consider here the case of a partial friction, where the liquid slips on the surface and prevent the viscous boundary layer to be fully developed.

To tune the friction, three types of surfaces are used: slippery multiscale super-hydrophobic surfaces, disordered super-hydrophobic surfaces (figure 1) and smooth hydrophilic surfaces. The spreading of drops (glycerol/water mixtures) on each surfaces is observed with a high-speed camera, and an automatic detection of the spreading time is performed (figure 2).

A model, taking into account the dynamics of the viscous boundary layer and the dynamics in the lamella, adapted from Roisman [2], is proposed to quantify this effect. The slip-length *b* can then be linked to the observed shift.

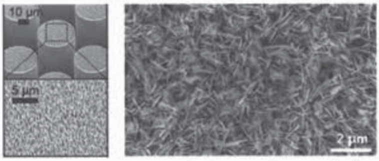

Figure 1 – Images of the surfaces. Left: slippery multiscale super-hydrophobic surfaces. Right: disordered super-hydrophobic surfaces.

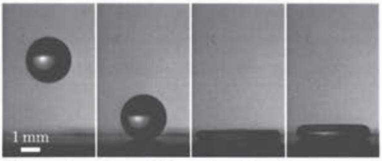

Figure 2 – Snapshots of a drop impact on a disordered super-hydrophobic surface (time interval 1 ms, $U = 1.47\ \mathrm{m/s}$*).*

References

[1] G. Lagubeau, Spreading dynamics of drop impacts, Journal of Fluid Mechanics **713**, 50-60 (2012)

[2] Illia V. Roisman, Inertia dominated drop collisions. II. An analytical solution of the Navier–Stokes equations for a spreading viscous film, Physics of Fluids **21**, 052104 (2009)

Localized self-assembly triggered by functionalized interfaces

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We will first present a simulation strategy allowing to model ligand-mediated interactions in systems with many colloidal particles. We will highlight how often the collective properties of the system are strongly affected by the timescales at which ligand-receptor linkages form and break. For instance, finite reaction rates drastically hamper relaxation towards equilibrium configurations resulting in more open aggregates when studying self-assembly [1], or fewer bound particles when considering targeting [2]. Finite reaction rates also favor rolling motion of interface bound particles [3].

We will then employ our framework to design a system in which functionalized interfaces initialize a cascade reaction leading to self-assembly of colloidal crystals with finite thickness [4]. Specifically, we will consider colloidal supported lipid bilayers functionalized by two types of complementary DNA sticky-ends. In bulk, intra-particle linkages prevent colloidal aggregation. In our system, the functionalized interface destabilizes intra-particle linkages and initiates self-assembly by magnifying particle-particle interaction. Importantly, our design provides full control over the crystal thickness and results in flat solid-fluid interfaces, a missing result in wetting theory.

References

[1] S. J. Bachmann, M. Petitzon, B. M. Mognetti, Soft Matter **12**, 9585 (2016)
[2] R. Lanfranco *et al*, Langmuir **35**, 2002 (2019)
[3] P. K. Jana, B. M. Mognetti, Phys. Rev. E, to appear, arxiv.org/abs/1907.11776
[4] P. K. Jana, B. M. Mognetti, Nanoscale **11**, 5450 (2019)

Electrolyte solutions at heterogeneously charged substrates

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The structure of a dilute electrolyte solution close to a surface carrying a non-homogeneous surface charge distribution are investigated by means of classical density functional theory (DFT) within the approach of fundamental measure theory (FMT). In the case of electrolyte solutions, the effects of these inhomogeneities are particularly severe due to the corresponding length scale being the Debye length, which is large compared to molecular sizes. A fully three-dimensional investigation is performed, which accounts explicitly for the solvent particles, and thus provides insight in effects of ion-solvent coupling. The present work introduces a powerful framework to study a broad range of possible surface charge heterogeneities even beyond the linear response regime, showing a sensitive dependence of the density profiles of the fluid components and of the electrostatic potential on the magnitude of the charge as well as on the short ranged details of the surface charge pattern.

Membrane close to critical demixing with a single inclusion

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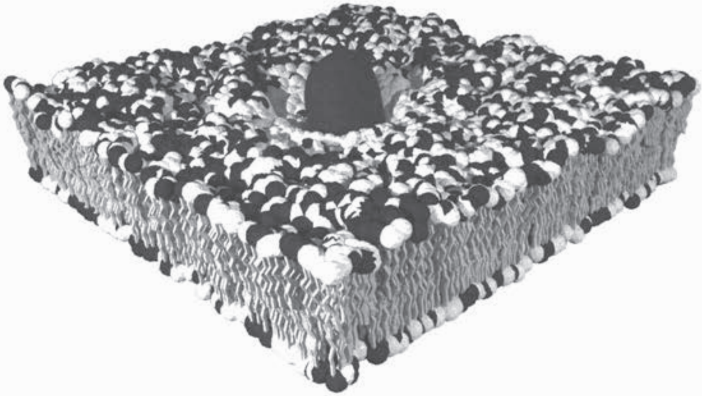

We present a simple model of a membrane described by two fluctuating fields: height above the flat surface and the chemical composition. Close to the critical demixing the membrane behaves as a flat sheet, while away from the criticality the composition degrees of freedom can be neglected. We study the response of such a system to a point defect (model of a protein) introduced on the membrane; we calculate the excess adsorption and the effective size of an induced deformation.

Synchronization in a binary mixture of brownian oscillators

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Synchronization phenomena are studied for a long time and are are present in many natural and artificial system, being the key studying phenomena in some of those[1,2].

In our work we try to understand how synchronization happens in a binary mixture of moving oscillators, in which similar oscillators try to synchronize and opposite ones try not too.

We do molecular dynamics simulation using an open-sour library (LAMMPS[3]) and we modify the Kuramoto model to apply it to our system, that is a binary mixture of particles, and where two similar particles try to have the same phase and two different particles try to have phases in the opposing direction. We simulate packing fractions, to see how the density contributes to the synchronization process.

If all particles have the same phase frequency it's always possible to achieve synchronization, and the presence of the anti aligning process enhances synchronization if the system is dense and hinders it if it is not.

References

[1] D. Levis, I. Pagonabarraga, *Phys. Rev. X* ,**7**, 011028 (2017)
[2] V. H. P. Louzada, N. A. M. Araújo, *Scientific Reports,* **2**, Article number: 658 (2012) [3] S. Plimpton,J Comp Phys, **117**, 1-19 (1995).

Non-equilibrium correlations and forces in sheared fluids with or without quenching

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Spatial correlations in media (e.g., fluids) can give rise to fluctuation-induced forces (FIFs) on objects immersed in the medium. Equilibrium correlations in fluids are typically bounded by the correlation length. Out of equilibrium, conservation laws can extend correlations beyond this length, leading, instead, to algebraic decays. This mechanism has been shown to give rise to purely non-equilibrium FIFs, e.g., following temperature quenches in conserved fluids.

I will discuss our recent study [1] of the correlations and forces in fluids driven out of equilibrium simultaneously by quenching and shearing, both for non-conserved ("Model A") as well as conserved ("Model B") diffusive stochastic dynamics. We identify which aspects of the correlations are due to shear and quenching (or to simultaneously applying both), as well as the role of the system's correlation length and its compressibility. The presence or absence of conservation laws influences the steady state correlation function strongly.

We further compute non-equilibrium FIFs between colloidal inclusions embedded in the sheared medium, with or without quenching. Due to the spatial symmetry breaking induced by shear, a rich phenomenology emerges: the forces can be stronger or weaker than their counterparts in unsheared systems, and generally do not point along the axis connecting the inclusions.

We expect our findings to be relevant for experimental systems where quenches or shearing are realizable, including active matter.

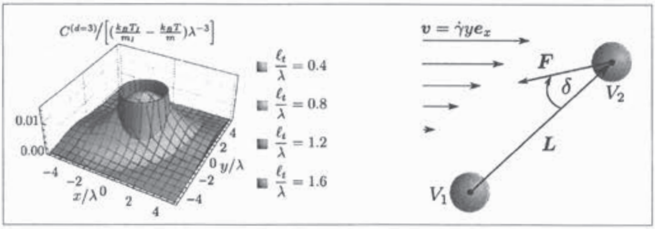

Fig. 1.
Left: The post-quench correlation function at different times, distorted by shear. Right: Spherical inclusions (e.g., colloids), immersed in the sheared fluctuating medium, for which we compute fluctuation-induced forces.

Left: The post-quench correlation function at different times, distorted by shear. Right: Spherical inclusions (e.g., colloids), immersed in the sheared fluctuating medium, for which we compute fluctuation-induced forces.

References

[1] C.M. Rohwer, A. Maciolek, S. Dietrich, and M. Krüger: New Journal of Physics **21**, 073029 (2019)

Wetting of Nematic Liquid Crystals on Crenellated Substrates: A Frank–Oseen Approach

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We revisit the wetting of nematic liquid crystals in contact with crenellated substrates, studied previously using the Landau–de Gennes formalism [1]. However, due to computational limitations, the characteristic length scales of the substrate relief considered in that study limited to less than 100 nematic correlation lengths. The current work [2] uses an extended Frank–Oseen formalism, which includes not only the free-energy contribution due to the elastic deformations but also the surface tension contributions and, if disclinations or other orientational field singularities are present, their core contributions. Within this framework, which was successfully applied to the anchoring transitions of a nematic liquid crystal in contact with structured substrates [3,4,5], we extended the study to much larger length scales including the macroscopic scale. In particular, we analyzed the interfacial states and the transitions between them at the nematic–isotropic coexistence.

References

[1] N. M. Silvestre, Z. Eskandari, P. Patrício, J. M. Romero-Enrique and M. M. Telo da Gama, Phys. Rev. E **86**, 011703 (2012).

[2] O. A. Rojas-Gómez, M. M. Telo da Gama and J. M. Romero-Enrique, Crystals **9**, 430 (2019).

[3] J. M. Romero-Enrique, C.-T. Pham and P. Patrício, Phys. Rev. E **82**, 011707 (2010).

[4] O. A. Rojas-Gómez and J. M. Romero-Enrique, Phys. Rev. E **86**, 041706 (2012).

[5] O. A. Rojas-Gómez and J. M. Romero-Enrique, J. Phys.: Condens. Matter **29**, 064002 (2017).

Capillary dynamics of a four-phase contact point

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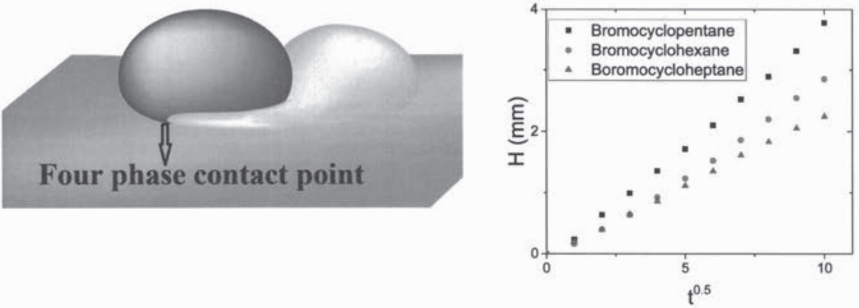
A four-phase contact point, e.g., in merging of immiscible drops, is the point where the liquid-liquid interface advances along the contact line of one drop. The dynamics of drop merging involve various driving and dissipating forces in the dynamics of the four-phase contact point. The viscous friction, i.e. the flow field, within liquids is influenced by the different boundary conditions on the different interfaces (liquid-gas, liquid-liquid, liquid-solid). Additionally, Marangoni stresses between the two liquids and the spreading coefficients along the contact lines play a role. Effectively, these effects lead to a capillary force acting on the four-phase contact point. In total, the situation resembles the capillary flow in open V-shaped groove. The important difference is that, in classical problem, the grooves are made out of two solid walls, but in the present case one of the "walls" is liquid (Fig.1 (a)). We investigate a range of liquids with different combination of physical properties (viscosity ratio, surface and interfacial tensions). The results show a good qualitative agreement for different liquids between the experimental results and classical Washburn equation ($h \sim \sqrt{t}$), which h is the capillary filled length by the second drop (Fig.1 (b)).



a

b

Fig. 1: a: Schematic of capillary rise problem of four pase contact point during drop merging process. b: sample results for pairs of water with Bromocyclopentane, Bromocyclohexane and Bromocycloheptane.

Hot active Janus colloids in a binary solvent

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Laser illuminating a Janus colloid which is suspended in a near-critical binary solvent leads to the formation of the concentration gradient and coarsening patterns around the colloid, which leads to its phoretic motion. Using analytical theory and numerical simulations, we investigate this non-equilibrium phenomenon under the influence of a time-dependent temperature gradient. Time-dependent properties of the coarsening patterns for various surface adsorption properties of the Janus colloid are analyzed. We also present results for the motion of the Janus colloid for various surface wetting properties, illumination intensity and surface adsorption properties.

Plasma-assisted growth of polyethylene fractal nano-islands on polyethylene oxide thin films

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Plasma-assisted vapor deposition of $(-CH_2-)_{100}$ macromolecules performed onto polyethylene oxide (PEO) nanolayers leads to formation of two-dimensional 7 nm thick polyethylene (PE) islands of the diverse fractal or dendrite shapes. AFM-infrared nanospectroscopy confirms the phase separation of PE and PEO, and illustrates microscopic details of fractal branches. The nanocalorimetry indicates that crossovers between island shapes may be related to chain dynamics in the PEO underlayer. On ultrathin (< 30 nm) PEO, star-shaped PE dendrites are observed. For thicker (~100 nm) PEO, the PE islands resemble the diffusion-limited aggregation fractals. The segmental mobility in PEO can be controlled by cross-linking which is enhanced under higher discharge power resulting in more linear backbone fractals. The results provide a new physical insight into solvent-free macromolecular diffusion at vacuum-polymer interface and may stimulate the vacuum-compatible development of new functional polymeric structures.

References

[1] A. Choukourov *et al.*, *Appl. Surf. Sci.* **489**, 55 (2019)

Artificial Chromatophores: Light-Triggered Nanoparticles for Microdroplet Locomotion and Color Change

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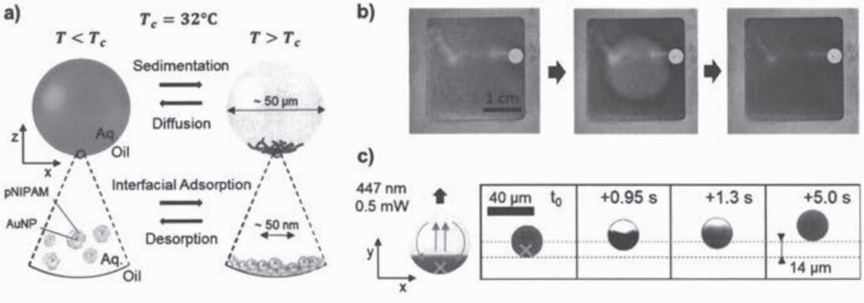
Gold nanoparticles coated with a poly(N-isopropylacrylamide) (pNIPAM) shell undergo reversible dis/assembly below and above the lower critical solution temperature of 32°C.[1] Loading these particles into aqueous microdroplets at high density creates light-driven artificial chromatophores.[2] Triggering the nanoparticle assembly gives dramatic color changes from nanoparticle localization at the base of the droplets, resembling zebrafish melanophores. These reversible chromatophore states can be switched by both bulk and optical heating, explored here in individual microdroplets and in large cm^2 areas of close-packed droplets. Illuminating chromatophores off-center with a tightly focused beam results in droplet locomotion via two separate mechanisms, Marangoni interfacial shear and gas bubble propulsion, depending on optical power.



a) Schematic temperature response of Au@pNIPAM core-shell nanoparticle loaded microdroplets. b) Color switching of a microdroplet film. c) Marangoni shear-induced droplet locomotion.

References

[1] T. Ding, V. Valev, A. R. Salmon, C. J. Forman, S. K. Smoukov, O. A. Scherman, D. Frenkel, J. J. Baumberg, PNAS **113**, 5503 (2016)

[2] A. R. Salmon, S. Cormier, W. Wang, C. Abell, J. J. Baumberg, Advanced Optical Materials, 1900951 (2019)

Filling transitions of a partially miscible binary liquid on a nanosculptured surface

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Abstract

A symmetric binary liquid mixture of species A and B is considered which is in contact with a wall endowed with nano pits. A situation is studied in which the liquid separates into an A rich liquid L_{A} and a B rich liquid L_{B} and furthermore one of the two species, say B, is attracted more strongly by the wall than the other. Thermodynamic conditions are chosen such that the space above the wall is filled with the liquid L_{A}, whereas the pits might be filled with L_{B}. By changing composition and packing fraction (density) in the L_{A} liquid above the wall it is possible to switch between two states in which the pits are either filled with L_{B} or L_{A}. A theoretical study of the switching behavior, including hysteresis, has been carried out using nonlocal classical density functional theory. The dependence of the switching behavior on the fluid–wall interactions and on geometric parameters is quantified.

Memory effects in polymer brushes showing co-nonsolvency effects

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Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. Previous studies focused on the response of brushes which are entirely covered by a liquid. Here, we concentrate on partial wetting of co-nonsolvent polymer brushes, i.e., on the dynamics of a three-phase contact line moving over such brushes. We demonstrate that the wetting behavior depends on the wetting history of the polymer brush.

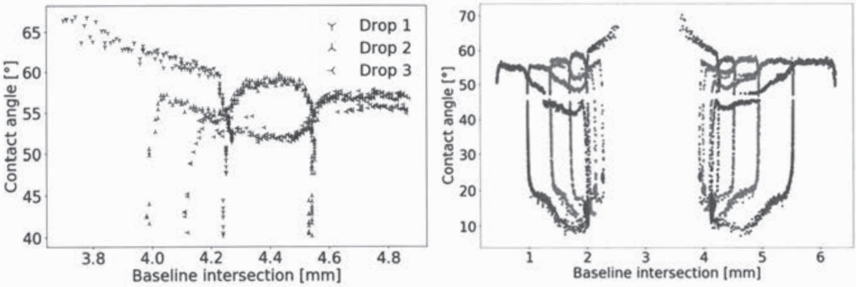

Figure 1: Change in contact angle through subsequent placed drops

We use Poly(N-isopropylacrylamide) (PNiPAAm) brushes and water and ethanol as good solvents. In water/ethanol mixtures, the brush thickness is a non-monotonous function of the ethanol concentration. The memory of brushes is tested by consecutively depositing drops of increasing size at the same position. Previously deposited drops induce changes in the brush that modifies the wetting behavior (advancing contact angle) of subsequent drops.

We believe that the change in the contact angels is induced by adaptation like swelling of or liquid exchange in the brush due to the drop on top. Also we investigate how different treatments of the brush changes the behavior of afterwards performed wetting experiments. Here the interaction of the moving 3 phase contact line with the brush is taken into account.

A study of metastability in hydrophobic surfaces

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The study of wetting phenomena in solids is of great interest due to the possible technological applications of hydrophobic and hydrophilic surfaces. Besides these applications, there are some fundamental open questions concerning the transition between these two wetting states. For instance, it is known that metastability is a common feature in experiments and that these metastable states are, in general, hydrophobic states. It is then important to understand what are the properties of the substrates that leads to this effect. In previous works, we have studied such phenomena using the analytical global energy approach and Monte Carlo simulations of the Cellular Potts model. We have compared the two methods for a wide variety of surface geometries and distinguish the results between the Wenzel (W) and Cassie-Baxter (CB) states, which are defined by the degree of wettability of the surface.

It has been shown that the final configuration depends strongly on the choice of initial wetting state of the droplet, which suggests the existence of a metastable regime in the system. To analyze systematically and understand this effect, in this work we apply a technique called Umbrella Sampling, that consist on adding a constraining term to the Hamiltonian, which drives the system to visit several specific configurations. We then use the results to calculate the free energy profile. This allows us to relate the energy barriers that lead to metastable states to the topology of the surface, which is a key point to understand the transition between CB and W states.

Hydrophobicity of surfaces in active matter

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Due to the formation of interfacial slip layers surfaces are of immense importance in active matter.[1,2] Both, the substrate as well as the particle surface are tuneable in terms of hydrophobicity through chemical functionalization. While the macroscale properties are easily accessible through contact angles, the colloidal nature makes the evaluation of hydrophobicity on the particle rather difficult. Here, we evaluate the effect of chemical functionalization on both, substrates as well as colloidal particles. We hypothize that the hydrophobic nature might enable selective interactions with passive particles.[3]

[1] J Simmchen, J Katuri, WE Uspal, MN Popescu, M Tasinkevych,Topographical pathways guide chemical microswimmers, Nature communications 2016, 7, 10598.

[2] L Wang, MN Popescu, F Stavale, A Ali, T Gemming, J Simmchen, Cu@ TiO 2 Janus microswimmers with a versatile motion mechanism, Soft matter 2019, 14 (34), 6969-6973.

[3] L Wang, J Simmchen, Interactions of Active Colloids with Passive Tracers, Condensed Matter 2019, 4 (3), 78.

Action at a distance in classical uniaxial ferromagnetic arrays: exact results and wetting effects

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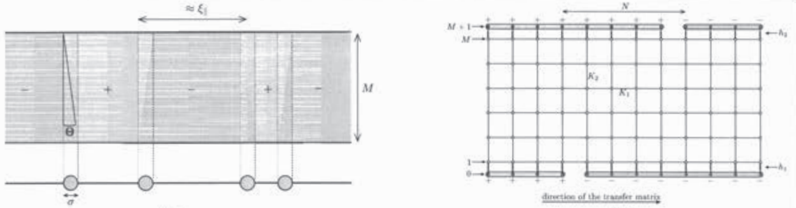
Can order extend over distances larger than the bulk correlation length? It has been shown in [1,2] that a network of Ising boxes connected by channels is able to exhibit an extraordinarily long-range ferromagnetic order over distances which grow exponentially with the cross sections of the channels. The emergence of such a new length scale follows from an exact calculation based on the diagonalization of the transfer matrix for the square lattice Ising model. The network of boxes is then studied both in theory and through extensive Monte Carlo simulations. Successively, we extend the study initiated in [1] by examining the role of wetting channels (fig. (a)). Domain walls inside channels are characterized by a finite contact angle (figs. (a) and (b)) and a point tension which diverges logarithmically upon approaching the wetting transition.



(a) (b)

References

1. D. B. Abraham, A. Maciołek, and O. Vasilyev, Phys. Rev. Lett. **113**, 077204 (2014).
2. D. B. Abraham, A. Maciołek, A. Squarcini, and O. Vasilyev, Phys. Rev. E **96**, 042154 (2017).
3. D. B. Abraham, A. Maciołek, and A. Squarcini, *to appear.*

The interface of the 3D Ising model and the vortex line in the 3D XY model: exact analytic results and numerical simulations

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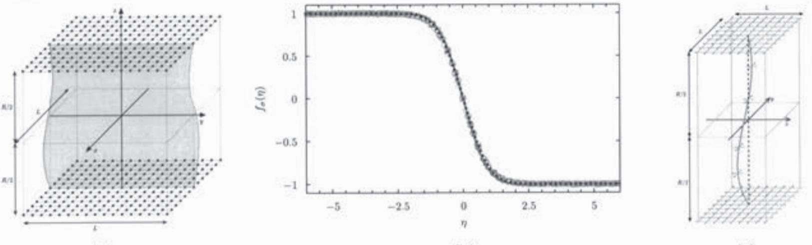
We show how recently developed field theoretical methods yield the exact determination of the order parameter profile and energy density for an interface in the 3D Ising model (figs. (a) and (b)) and for a topological vortex line in the 3D XY model (fig. (b)). Our analytical results are in complete agreement with high-precision Monte Carlo simulations we performed.



(a) (b) (c)

References

4. G. Delfino, W. Selke, and A. Squarcini, Phys. Rev. Lett. **122**, 050602 (2019).
5. G. Delfino, W. Selke, and A. Squarcini, *submitted to Journal of High Energy Physics.*

The shape of liquid bridges

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We have studied a single vertical, two-dimensional liquid bridge spanning the gap between two flat, horizontal solid substrates of given wettabilities. For this simple geometry, the Young-Laplace equation can be solved (quasi-)analytically to yield the equilibrium bridge shape under gravity. We establish the range of gap widths (as described by a Bond number Bo) for which the liquid bridge can exist, for given contact angles at the top and bottom substrates (θ_c^t and θ_c^b , respectively). In particular, we find that the absolute maximum span of a liquid bridge is four capillary lengths, for $\theta_c^b = 180°$ and $\theta_c^t = 0°$; whereas for $\theta_c^b = 0°$ and $\theta_c^t = 180°$ no bridge can form, for any substrate separation. We also obtain the minimum value of the cross-sectional area of such a liquid bridge, as well as the conditions for the existence and positions of any necks or bulges and inflection points on its surface. This generalises our earlier work in which the gap was assumed to be spanned by a liquid film of zero thickness connecting two menisci at the bottom and top substrates.

Dynamics of particles confined by droplets

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Droplet confined solid particles are called compound particles. These are often encountered in a variety of situations, for e.g. nucleated cells, aerosols, droplet-based encapsulation of motile organisms, polymer microcapsules, particle stabilized emulsions, etc. In this study, we investigate the hydrodynamics of a compound particle. Assuming small Capillary number, analytical solutions are obtained to describe the dynamics of a compound particle when the particle and the drop have a concentric configuration. Concentric configuration of a translating compound particle is found to be not a steady-state configuration. This happens since the confining droplet does not move with the same velocity as that of the driven particle. The effect of size of the confining surface and viscosity of both the confining fluid and the dispersed fluid are also analyzed. Finally, we study the dynamics of a compound particle in common ambient flows - simple shear, uniaxial, and biaxial flows and provide a comprehensive comparison on the effect of ambient flows on the stability of compound particles. We propose a mechanism to stabilize the configuration by a square wave shear input [1]. Finally we extend the studies by considering active particles entrapped in the droplet.

References

[1] Venkata, S.C.K. and Thampi, S.P., 2019. Dynamics and stability of a concentric compound particle-a theoretical study. *Soft matter*.

The triple line tension of water in extreme confinement

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Wetting at the nanoscale is a topic of paramount physical and technological importance: as the lengthscale approaches the nanometer, (e.g. in confinement) peculiar features emerge, crucial to a number of phenomena spanning from physics to biology to material science. Examples include the accelerated drying of water in hydrophobic nanopores [1-3], in planar confinement [4] and at the interface between biological macromolecules [5].

The triple line tension, owing to its linear scaling, is widely used to pro- vide a simple continuum modeling of such nanoscale deviations from the macroscopic behaviour, otherwise ruled by the interplay of surface and volume scaling terms [3-4]. Nevertheless the line tension of water remains an elusive quantity that is very hard to directly probe in experiments and simulations. The lack of a comprehensive nucleation theory capable of interpreting experimental or simulation data results in the absence of a definitive consensus on the magnitude or sign of the line tension.

In this contribution, using a combination of free energy molecular dynamics simulations and continuum modeling, we are able to provide estimates of the line tension of water on model substrates, to discuss its importance in nanoscale accelerated evaporation and to highlight the role of the geometry and of the confinement on the triple line tension. This effort also allows us to interpret available experimental and simulation data.

This project has received funding from the European Research Council under the European Union's Seventh Framework Program (FP7/2007–2013)/ERC Grant Agreement 339446 and European Unions's Horizon 2020 research and innovation agreement No.803213

References

1. Tinti et al. (2017). Intrusion and extrusion of water in hydrophobic nanopores. Proceedings of the National Academy of Sciences, 114(48), E10266-E10273.

2. Tinti et al. (2018). Vapor nucleation paths in lyophobic nanopores. The European Physical Journal E, 41(4), 52.

3. Guillemot et al. (2012). Activated drying in hydrophobic nanopores and the line tension of water. Proceedings of the National Academy of Sciences, 109(48), 19557-19562.

4. Sharma and Debenedetti, (2012). Evaporation rate of water in hydrophobic confinement. Proceedings of the National Academy of Sciences, 109(12), 4365-4370.

5. Zhou et al. (2004). Hydrophobic collapse in multidomain protein folding. Science, 305(5690), 1605-1609.

Non-equilibrium effects of the wetting properties at switchable substrates

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The wetting behavior of reversibly switchable surfaces can be changed in a wide range which is useful for many applications like microfluidics and printing processes. These surfaces are built for example out of azobenzenes which can be switched from a cis to a trans state with light of a defined wavelength.

We investigate the behavior of liquids on these surfaces from a theoretical perspective. For this purpose, we consider a droplet consisting of Lennard-Jones particles on a fcc lattice. By changing the interaction strength between the substrate and droplet particles the wetting behavior can be controlled. We study two different aspects via Molecular Dynamics Simulations. (1) By fast switching of the interaction strength we impose a non-equilibrium behavior on the shape of the droplet. Specific features are observed which significantly differ from the equilibrium behavior. (2) We systematically calculate for different interaction strengths the interface tensions between the solid, liquid and gas phase as well as the interface potential existing for thin films of liquids. This can be used as input for a continuum description of these non-equilibrium processes.

Hourglasses at a fluid-fluid interface: multipoles, demixing and hindered assembly

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The function of colloidal particles–typically determined by their chemical composition–can be enhanced significantly by their shape and structure. 2D structures of colloidal particles can be obtained by letting particles self-assemble at a fluid-fluid interface. For all but the smallest of particles, this assembly is driven primarily by capillary forces. In this work, we investigate the adsorption, capillary interactions and self-assembly of hourglass-shaped particles using a combination of numerical methods. By calculating the energetics of the particle adsorbing onto the fluid-fluid interface, we find there are two modes in which it adsorbs: horizontal and vertical. By taking into account how the fluid-fluid interface is deformed by the adsorbed particle, we find that the two different modes induce different capillary interactions: horizontally adsorbed particles are capillary quadrupoles, while vertically adsorbed ones are (weak) capillary monopoles. Many-particle simulations with approximated versions of these interactions then reproduce multiple phenomena seen in the experimental self-assembly: demixing of the two adsorption modes, the formation of string-like structures and the unexpectedly low fraction of densely packed crystalline regions. Our work demonstrates that a complex particle shape can induce complex capillary behaviour, but that relatively simple numerical methods are already quite effective at capturing these new phenomena.

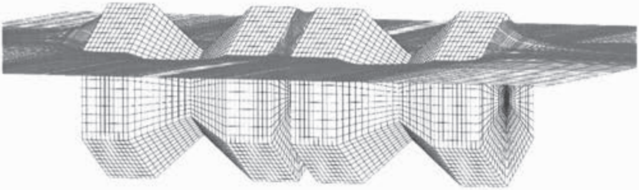

Figure 1: Simulated capillary deformation between two horizontally adsorbed hourglass particles. The deformation of the interface subsequently induces capillary many-body interactions, which drive the self-assembly.

Bridging transition between particles

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Let us consider a binary liquid mixture below the critical point. Colloid particles, which prefer the component of the mixture opposite to that favored in the bulk, are immersed into the binary mixture. In such system capillary bridge appear between colloids at short separations. Computer simulations for the Ising model are performed in order to investigate conditions of capillary bridges formation.

PACS numbers: 05.70.Jk, 64.60.Ak, 05.10.Ln

References

[1] *Nonadditive interactions and phase transitions in strongly confined colloidal systems,*
Oleg A. Vasilyev, S. Dietrich, and Svyatoslav Kondrat, Soft Matter **14** 586 (2018)
[2] *Bridging transitions and capillary forces for colloids in a slit,*
O.A. Vasilyev, M. Labbé-Laurent, S. Dietrich, and S. Kondrat, in preparation

Surface wettability-induced sign inversion of the apparent line tension in sessile nanodroplets

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Despite strenuous research efforts for more than one century, identifying the magnitude and sign of the apparent line tension for a liquid-solid-gas system remains an elusive goal [1-4]. Herein we accurately determine the apparent line tension from the size-dependent contact angle of sessile nanodrops on surfaces with different wetting properties via atomic force microscopy measurements and molecular dynamics simulations. We show that the apparent line tension has a magnitude of 10^{-11}-10^{-10} J/m $10^{-11} - 10^{-10}\ \mathrm{J/m}$, in good agreement with theoretical predictions. Furthermore, while it is positive and favors shorter contact lines for droplets on very lyophilic surfaces, the apparent line tension changes its sign and favors longer contact lines on surfaces with an apparent contact angle higher than a critical value. By analyzing the density and the potential energy of liquid molecules within the sessile droplet, we demonstrate that the sign of the apparent line tension is a thermodynamic property of the liquid-solid-gas system rather than the local effect of intermolecular interactions in the three-phase confluence region [5].

References

[1] L. Schimmele, M. Napiórkowski, and S. Dietrich, The Journal of Chemical Physics **127**, 164715 (2007).

[2] J. H. Weijs, A. Marchand, B. Andreotti, D. Lohse, and J. H. Snoeijer, Physics of Fluids **23**, 022001 (2011).

[3] J. Zhang, P. Wang, M. K. Borg, J. M. Reese, and D. Wen, Physics of Fluids **30**, 082003 (2018).

[4] M. Kanduč, L. Eixeres, S. Liese, and R. R. Netz, Physical Review E **98**, 032804 (2018).

[5] B. Zhao, S. Luo, E. Bonaccurso, G. K. Auernhammer, X. Deng, Z. Li, and L. Chen, Physical Review Letters **123**, 094501 (2019).