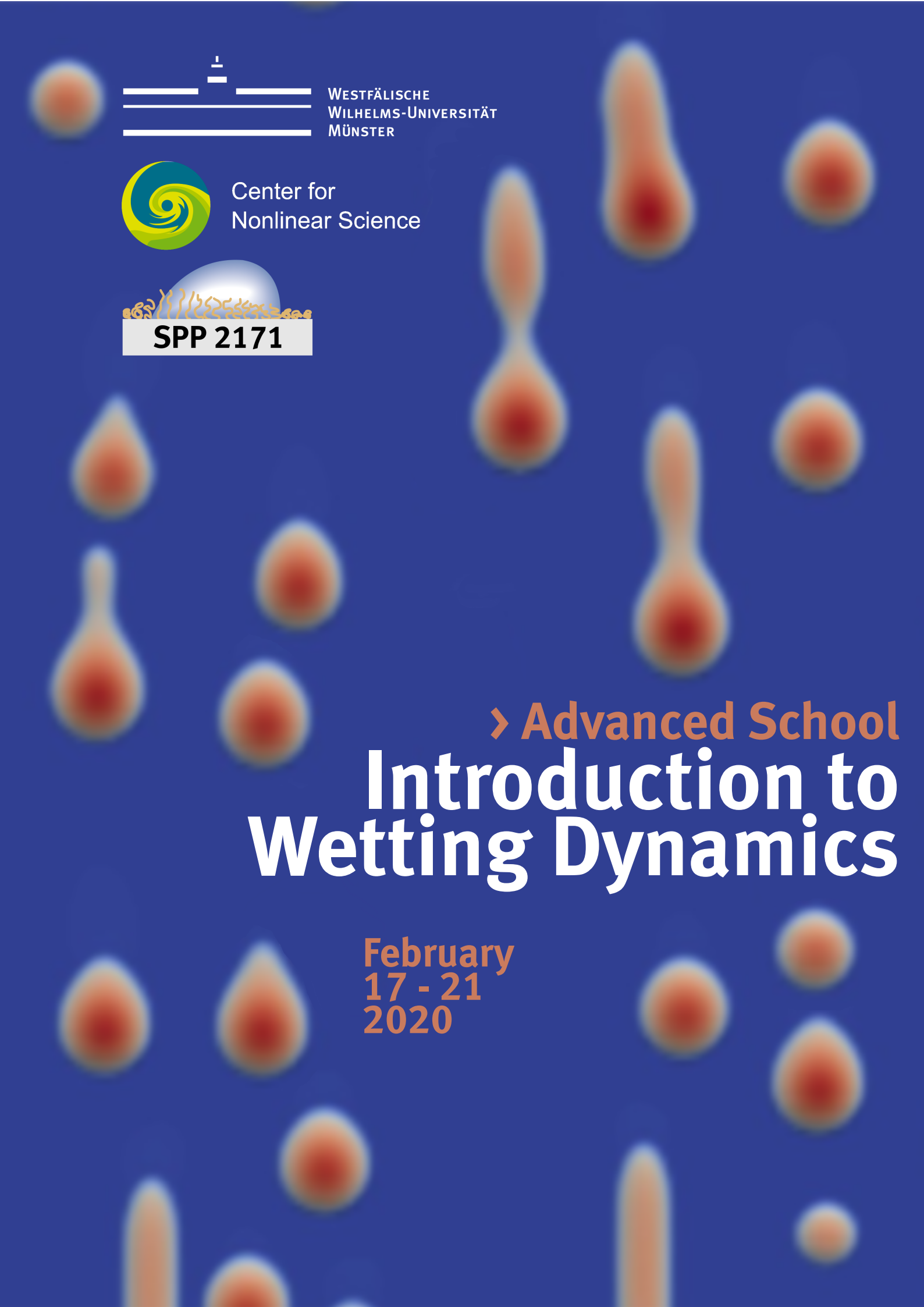
Westfälische
Wilhelms-Universität
Münster
Center for
Nonlinear Science
SPP 2171
› Advanced School
Introduction to
Wetting Dynamics
February
17 - 21
2020

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LOCATION

The workshop takes place in lecture hall 404 of the

Institut für Theoretische Physik
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Wilhelm-Klemm-Straße 9
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Lunch and coffee is served in rooms 303 and 304.

INTRODUCTION TO WETTING DYNAMICS

The Advanced Winter School "Introduction to Wetting Dynamics" shall introduce Master students, PhD candidates and more senior researchers into the themes underlying the Priority Programme 2171 "Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates". In particular, introductions are given to wetting and dewetting processes on static surfaces as well as on surfaces with intrinsic dynamics. For instance, flexible surfaces are deformed by the liquid and thus provide a feedback mechanism and switchable surfaces can repeatedly and almost instantaneously change their surface energy or topography in response to external influences. Both, experimental and theoretical methods are introduced that allow one to tackle the involved multiscale processes. Examples include novel visualisation methods as confocal laser-scanning-microscopy and x-ray tomography and a spectrum of simulation methods for microscopic, mesoscopic and macroscopic models.

The School combines long tutorial lectures with shorter presentations by an interdisciplinary group of experts across the fields of physico-chemical hydrodynamics, statistical physics, surface science, chemical physics and various engineering disciplines. A poster session allows participants to present and discuss their results.

MONDAY, FEBRUARY 17, 2020

PROGRAM

12.00	Registration and coffee	
13.00	Wetting and dewetting phenomena: physical concepts, experimental evidences, and theoretical modeling	**R. Seemann**
14.30	Coffee	
15.00	Introduction to the Theory of Wetting	**M. Müller**
16.45	Welcome buffet and posters	
18.30	End	

Ralf Seemann Saarland University

Wetting and dewetting phenomena: physical concepts, experimental evidences, and theoretical modeling

We will provide an introduction to (de-) wetting phenomena of thin film liquid films from solid substrates. Particular emphasis will be on van der Waals forces that can destabilize nanoscopic thin films by spinodal dewetting and how these hole nucleation process can be distinguished from heterogeneous nucleation. Moreover, we will also show how van der Waals forces influence the liquid profiles close to the three phase contact line and the effective contact angle of nanoscopic droplets. If time allows we will further shed light on the dewetting process subsequent to hole formation and the characteristic rim shapes that emerge as function of slip at the liquid solid interface when the dewetting liquid is removed from the dry spot.

Marcus Müller Georg-August University Göttingen

Introduction to the Theory of Wetting

This lecture will provide a basic introduction in the theory of wetting. Starting out with a simple description of an interface between coexisting phases, we will derive the interface potential and basic thermodynamic and dynamic aspects of wetting phenomena. Particular emphasize will be devoted to the relation between macroscopic properties of a continuum description (e.g., contact angle) and microscopic interactions between the constituent particles of the liquid, as well as technique that establish such a quantitative relation by computer simulation. These aspects will be exemplified by simulations of polymer liquids.

Gulzar Ahmad University of Freiburg

Poster: Evaluation of droplet shape and three-phase contact line movement on dynamically switchable spiropyran surfaces

Wetting, the spreading of liquids on solid surfaces is of high interest for many processes in science and everyday life. It is generally agreed that the properties of the solid substrate have a significant influence on the wetting behaviour. For the behaviour of droplets the three-phase contact line, the line where liquid, solid and gas phase meet plays a major role. Surface heterogeneity only impacts the macroscopic behaviour of the droplet if it is situated under the three-phase contact line. The experimental evaluation of the dynamics of this line is therefore of great interest. In this project, the influence of substrate dynamics on the behaviour of droplets will be investigated. The main focus of this project is the analysis of the three phase contact line. In the course of this project dynamic substrates which can be switched between different states of surface energy (hydrophilic/ hydrophobic) based on spiropyrans will be generated and analysed in terms of their switching properties. Spiropyran surfaces are advantageous because the switch is directly visible due to a colour change from colourless (hydrophobic) to an intense magenta colouring (hydrophilic). For the fabrication of such substrates, processes for the generation of micro/nanostructured polymer foams in combination with spiropyran immobilization via photobleaching can be employed. Additionally, new spiropyran-copolymer mixtures and polymers with spiropyran-crosslinkers will be used. An imaging platform consisting of two highspeed cameras in combination with a maskless lithography setup for the generation of switching patterns will be set up for analysing the droplets during and after the switch.

Niklas B. Arndt WWU Münster
Natalie Harmeyer, Friederike Schlüter and Bart Jan Ravoo

Poster: Dynamic Wetting of Self-Assembled Monolayers functionalised with Photoresponsive Arylazopyrazoles

Light is a particularly attractive external stimulus to modify surface properties since it can be applied with very high local and temporal resolution. Molecular photoswitches such as azobenzenes,[1] diarylethenes[2] and spiropyranes[3] have been explored in a range of photoresponsive coatings which utilize their photoisomerization to induce changes in macroscopic properties such as wettability.[4] Especially azobenzenes have been immobilized on a variety of sur-

faces to obtain photoswitchable wettability since the trans-isomer is much less polar than the open cis-isomer. This results in a substantial and reversible change of wettability.[5] Current approaches using immobilized photoswitches still suffer from certain drawbacks. Diarylethenes and spiropyranes display poor fatigue resistance while azobenzenes exhibit a significant overlap of the bands for trans- and cis-isomer. This overlap results in only about 50 % of the switches effectively changing conformation upon irradiation.[1] Arylazopyrazoles (AAPs) in contrast offer significant improvements of these photophysical properties. Methylsubstituted APPs exhibit a much more favorable photostationary state (> 98 % in both directions), very slow thermal relaxation of the cis-isomer towards the thermodynamically favored trans-isomer and very good fatigue resistance.[6] Therefore, the immobilization of AAPs on surfaces using self-assembled monolayers (SAMs) is predicted to yield surfaces featuring photoresponsive wetting behavior which shows low cycling fatigue and a significant improvement to the photostationary state. Herein we report the synthesis of an AAP-silane derivative and the successful functionalization of quartzglas surfaces using self-assembled monolayers of this silane derivative. The dynamic wetting abilities are demonstrated using contact angle measurements. Furthermore we present DFT calculations of possible APP derivatives exhibiting different levels of polarity change upon photoisomerization.

[1] Bandara, H. M. D.; Burdette, S. C. Photoisomerization in different classes of azobenzene. Chem. Soc. Rev. 2012, 41, 1809-1825.
[2] Tian, H.; Yang, S. Recent progresses on diarylethene based photochromic switches. Chem. Soc. Rev. 2004, 33, 85-97.
[3] Klajn, R. Spiropyran-based dynamic materials. Chem. Soc. Rev. 2013, 43, 148-184.
[4] Xin, B.; Hao, J. Reversibly switchable wettability. Chem. Soc. Rev. 2010, 39, 769-782.
[5] Groten, J.; Bunte, C.; Rühe, J. Light-induced switching of surfaces at wetting transitions through photoisomerization of polymer monolayers. Langmuir : the ACS journal of surfaces and colloids 2012, 28, 15038-15046.
[6] Weston, C. E.; Richardson, R. D.; Haycock, P. R.; White, A. J. P.; Fuchter, M. J. Arylazopyrazoles: azoheteroarene photoswitches offering quantitative isomerization and long thermal half-lives. Journal of the American Chemical Society 2014, 136, 11878-11881.

Lauritz Beck Technische Universität Darmstadt

Poster: Highly accurate numerical simulation of wetting, dewetting and fluid-splitting phenomena between elastic surfaces

We present a highly accurate extended discontinuous Galerkin (XDG) method to simulate the interaction of liquids with flexible substrates. Utilizing the strongly coupled approach proposed by Matthies and Steindorf [1], we combine existing solvers for multiphase flows with contact lines and structural solvers. Since this approach allows to reuse existing solvers, the XDG solver for multiphase flows with contact lines developed by the authors is applied [2]. This solver allows a sharp representation of the liquid-gaseous interfaces as well as singular forces to model contact line dynamics. The solid phase is solved by an off-the-shelf structural solver, adding flexibility to the method. We conduct numerical simulations to investigate how the replacement of effects which are beyond continuum physics by numerical artifacts compromise the simulationsâ overall validity. Since the simulations mirror experiments within the Priority Programme, we expect to gain qualitative and quantitative insight into flow details not visible for measurement in the region of contact lines.

[1] Matthies, H., Steindorf, J., 2003. Partitioned strong coupling algorithms for fluid-structure interaction, Computers Structures, Volume 81, Issues 8-11, 805-812

[2] Kummer, F., 2017. Extended discontinuous Galerkin methods for two-phase flows: the spatial discretization. Int. J. Numer. Meth. Engng, 109: 259-289.

Vishal Dadhich Technische Universität Darmstadt

Poster: Determining the location of hydrodynamic boundary using mode analysis method

Navier Stokes equation, unlike Maxwell equations, requires prior knowledge of boundary conditions in-order to solve it. Due to this, determining the hydrodynamic boundary has been a fundamental problem. This becomes more crucial in understanding the dynamics of nanofluidic systems where the interfacial fluid structure becomes more critical. Based on Green Kubo relations, couette and poiseuille flows, There are many popular approaches used to understand the dynamics of such systems. These methods usually approximate or in some cases ignore the presence of a hydrodynamic boundary layer. In this poster, I will be discussing an alternate approach to this problem, intro-

duced by Chen et al (2015). Mode analysis method allows us to precisely locates the hydrodynamic boundary in small confined systems. This is achieved by identifying thermally excited hydrodynamic modes and their relaxation times in equilibrium. This approach also lets us measure the slip length and coefficient of viscosity which also leads to calculation of surface frictional coefficient. Alongside the method itself, I will also discuss some preliminary results of different systems.

Kirsten Harth Otto-von-Guericke-Universität Magdeburg

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

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.

Hansol Jeon MPI-DS Göttingen
and Stefan Karpitschka

Poster: Liquid-liquid phase separation in contact with deformable surfaces

The capillary forces of droplets on top of soft solids deform the solid surface into sharp wetting ridges. The amplitude of the wetting ridge is governed by elasto-capillary length, the ratio of liquid surface tension to the solidâs shear modulus. Previous experiments on soft wetting used large liquid-vapour surface tensions and thus were in a highly nonlinear regime regarding the response of the solid. This led to debates in the literature regarding the effects of strain dependent solid surface tensions or the dynamics of soft wetting. Liquid interfaces with small surface tensions could instead probe the linear regime of soft wetting and shed new light onto the static and dynamic behaviours of solid surface tension. Thus we investigate the liquid-immersed case of soft wetting, aiming for a control of the liquid and solid surface tensions. We tested various liquid combinations and explored a wide range of surface tensions and substrate shear moduli, finding valid Neumann constructions in all cases.

Nikolai Kubochkin TU Darmstadt

Poster: Modelling of Spreading, Imbibition and Evaporation of Liquids on Structured or Porous Deformable Substrates

Spreading and evaporation of liquids on surfaces and imbibition of liquids into porous layers are important processes for many natural phenomena and industrial applications. They have been a focus of numerous experimental and theoretical/numerical studies. The project aims to develop mathematical models for spreading, imbibition and evaporation of liquids on structured or porous deformable substrates. The thin film theory-based numerical model will be developed, validated and applied to elastic deformable substrates with shallow topography, whereas the full understanding of the influence of material, structural and process parameters on spreading, imbibition and evaporation processes will be achieved. In parallel, the wetting and evaporation of liquids on elements of deformable porous structure will be modelled numerically. As the first step, spreading of droplets over undeformable surfaces for complete and partial wetting cases have been studied.

Dominic Mokbel HTW Dresden

Poster: Efficient simulations of dynamic wetting of flexible substrates

Wetting of elastic substrates plays a major role in a broad variety of phenomena in nature and technology. Yet, the continuum modeling and simulation of soft wetting has remained essentially unexplored. In this project we combine phase-field modeling of two-phase flow with fluid-structure interaction to develop an efficient numerical framework for investigating some of the exciting phenomena encountered in soft wetting experiments.

Simon Schubotz IPF Dresden
Petra Uhlmann, Andreas Fery, Jens-Uwe Sommer, Günter K. Auernhammer

Poster: Memory effects in polymer brushes showing co-nonsolvency effects

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. 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 conclude 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. Additionally, we investigate how different ways of prewetting the brush change the following wetting experiments. We have hints that the interaction of the moving three-phase contact line with the brush has to be taken into account.

Lucia Wesenberg Georg-August-Universität Göttingen

Poster: Wetting of bio-inspired, stimulus-responsive polymer surfaces by lipid vesicles

The fabrication of switchable interlayers between soft, biological objects and hard solids is one of the major challenges to dynamically regulate the interfacial interactions. We will investigate the wetting of bio-inspired, stimulus-responsive polymer substrates by lipid vesicles both through experiments and by simulation. In analogy to the wetting by liquid drops, the shape of a vesicle is dictated by the enclosed volume, the membrane-substrate interaction (interface potential), and the properties of the interface (membrane) between the interior and exterior. Unique to wetting by flexible vesicles is the importance of the membraneâs bending rigidity in addition to its tension. The Tanaka group will fabricate and characterize stimulus-responsive substrates based on polymer brushes. The abrupt change in polymer conformation is followed by dynamic changes in the wetting behavior of lipid vesicles. The dynamic changes in the global shape of the vesicles, vesicle footprint, membrane height fluctuations, and hydrodynamics inside the vesicles will be monitored through various experimental techniques. The MÃŒller group will complement the experiments by simulations. To reach the spatio-temporal scales of the experiments, the switchable polymer brush is modeled by a highly coarse-grained particle model whereas the vesicle membrane will be represented by a triangulated sheet within the framework of the Helfrich Hamiltonian. This poster presents first results, including the effects of wall potential, radius, and triangulation on the equilibrium vesicle shape as well as the ion-selective switching of the interfacial potential.

PROGRAM

9.00	Statics and dynamics of soft wetting	**J. Snoeijer**
10.30	Coffee	
11.00	Solid-state wetting and dewetting	**O. Pierre-Louis**
11.45	Variational modeling of bulk and interface effects in fluid dynamics	**D. Peschka**
13.00	Lunch	
14.00	Drops on liquid impregnated slippery surfaces	**D. Vollmer**
15.30	Coffee	
16.00	Chemical tailoring of micro- and nanostructured surfaces to control wetting	**J. Rühe**
16.45	Surface stresses in soft gels	**R. Style**
19.00	Conference dinner at Schlossgarten	

Jacco Snoeijer University of Twente

Statics and dynamics of soft wetting

The laws of wetting are well known for drops on rigid surfaces but change dramatically when the substrate is soft and deformable. The combination of wetting and the intricacies of soft polymeric interfaces have provided many rich examples of fluidâstructure interactions, both in terms of phenomenology and from a fundamental perspective. In this review we 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.

Olivier Pierre-Louis Université Claude Bernard Lyon 1

Solid-state wetting and dewetting

During the 20th century, the theory of liquid-state wetting served as a basis to the study of micro- and nano-scale solids, notably by the Bulgarian school with Ivan N. Stranski, R. Kaischew, and others. The concept of solid-state wetting provided a rationale for the observation of different growth modes of thin solid films, leading sometimes to continuous films, and sometimes to assemblies of solid droplets. However, it was quickly understood that the wetting behavior of solids exhibits differences from that of liquids, because of the relevance of different physical ingredients such as elastic strain, anisotropy, and mass transport via surface diffusion.

Nowadays, while epitaxial growth is still a central tool to obtain thin films and nanoparticles on solid substrates, new ways to produce nanoscale solids at solid surfaces are known, such as nanoscale lithography, nanoparticle deposition, catalyzed nanowire growth, or direct bonding. These techniques allow one to produce a wide variety of nano-objects (islands, wires, films, etc.), which evolve not only during growth, but also under annealing while interacting with a substrate, thereby leading to wetting behaviors that are similar to those reported in modern liquid-state wetting studies. For example, the studies of the dynamics of spreading and dewetting, or of wetting on patterned surfaces, with the so-called Lotus effect exhibit some kind of counterpart in solid-state wetting.

Dirk Peschka WIAS Berlin

Variational modeling of bulk and interface effects in fluid dynamics

In the first part of my lecture I will introduce a thermodynamics inspired variational framework to model hydrodynamics of simple fluids with moving domains, interfaces, and contact lines. Based on rather generic expressions for energy and dissipation a very rich set of partial differential equations will emerge, where in particular the coupling of bulk and interface effects emerges in a natural way. In the second part of my lecture I will indicate several generalizations of this framework considering substrate dynamics and reversible processes.

Doris Vollmer MPI-P Mainz

Drops on liquid impregnated slippery surfaces

Textured substrates which are impregnated by a lubricant form a new class of functional surfaces, called slippery surfaces. Texture is key for capillary forces to lock the lubricant in place. Slippery surfaces can repel almost all types of liquids and are capable of healing physical damages by capillary wicking. Drops deposited on slippery surfaces roll off when tilting the surface by a few degrees. However, modelling of liquid impregnated surfaces is challenging because there are 4 phases at play: the solid texture, the impregnating lubricant, the surrounding vapor (air), and the aqueous drop. Characteristic is that sliding liquid or solid particles are surrounded by an annular wetting ridge. On the one hand this influences the wetting behaviour and can determine the friction a drop experiences on these surfaces. On the other hand the wetting ridge can cause depletion of lubricant, because lubricant is taken along with moving liquids. First: I'm going to discuss how to prepare liquid impregnated slippery surfaces. Next I will discuss relevant thermodynamic factors that influence the properties of lubricated surfaces. Moving drops experience friction. I will introduce various sources that can contribute to friction. Furthermore, I will discuss different techniques how to investigate slippery surfaces and the advantages and disadvantages of slippery surfaces in the context of prospective applications.

F. Schellenberger, J. Xie, N. Encinas, A. Hardy, M. Klapper, P. Papadopoulos, H.-J. Butt, D. Vollmer, Direct observation of drops on slippery lubricant-infused surfaces, Soft Matter 11, 7617 (2015).

Jürgen Rühe University of Freiburg

Chemical tailoring of micro- and nanostructured surfaces to control wetting

The wetting properties of a certain material like many other surface properties are determined by the "last few nanometers". This provides surface scientists with the unique opportunity to use ultrathin coatings to tailor surfaces in this regard. However, aside from the chemical properties of a surface, wetting is also largely controlled by topology. Extreme wetting cases – like superhydrophobic or superhydrophilic surfaces – require a non-planar, i.e. rough or structured surface topography. This rules out many typical coating strategies as these would alter the topography or even completely bury it underneath the coating material. In this contribution we will discuss several strategies to chemically modify surfaces with an emphasis on those techniques are best suited to tailor wetting properties.

Robert Style ETH Zürich

Surface stresses in soft gels

Surface stress, also known as surface tension, is a fundamental property of any interface. In stiff solids, it normally has a negligible effect. However, it can significantly affect the mechanical behaviour of soft solids. For example, I will show how it can completely change wetting, adhesion, and composite properties. I will also explain how we can characterise surface stresses in soft solids by examining the contact line of droplets on soft surfaces, or by looking at the equilibrium of patterned soft surfaces.

PROGRAM

9.00	Including thermal effects in modeling and computing dynamics of thin films	**L. Kondic**
10.30	Coffee	
11.00	Modelling and analysis of the swelling of driven hydrogels	**A. Münch**
11.45	Introduction to the gradient dynamics description for thin films	**S. Gurevich**
12.30	SPP 2171 – Activities and Opportunities	**U. Thiele**
13.00	Lunch	
14.00	Discussions and individual project meetings (open end)	

Lou Kondic New Jersey Institute of Technology

Including thermal effects in modeling and computing dynamics of thin films

This lecture will focus on modeling evolution of thin fluid films in setups where thermal effects are of relevance. In particular, we will discuss different ways in which thermal effects could be of relevance to dynamics of thin films, including spatial and temporal dependence of material parameters, such as viscosity, surface tension, or density. The second part of the lecture will focus on a films exposed to an external heat source on a thermally conductive substrates. The particular case that will be used as a motivation involves evolving metal films of nanoscale thickness exposed to external laser heating; however the mathematical models and supporting computations are more general and could be applied to a variety of materials and heating mechanisms. One challenge in considering films on thermally conductive substrates involves coming up with accurate models for evolution of thermal energy that could be efficiently coupled with the fluid mechanical evolution of the film itself. The talk will also touch on some new and not completely understood results including the possibility of oscillatory film instabilities, among others.

Andreas Münch University of Oxford

Modelling and analysis of the swelling of driven hydrogels

Hydrogels are two-phase systems composed of an elastic network of polymer chains penetrated by a solvent, inducing large deformations of the network as the gel swells and dries. They are ubiquitous in many biological processes and have a vast range of medical and also smart soft-matter applications and have been attracting a lot of attention. They are also attractive from a fundamental point of view due to their rich equilibrium structure as well as dynamic behaviour which involves pattern formation and phase transitions during swelling and drying. In this talk, we will present a derivation of a full kinetic model of a solvent-network hydrogel that undergoes phase separation, based on a full nonlinear treatment of the elastic network and thermodynamic consistency. The model accounts for the interfacial energy of co-existing phases, finite strain of the polymer network, and solvent transport across free boundaries, and we discuss the phase transitions via numerical and phase-plane methods. This system is then discussed using phase-plane analysis and numerical solutions in a 1D setting. We also discuss extensions to

polyelectrolyte gels and additional ionic species and the possibility of collapse induced by varying salt concentrations.

Svetlana Gurevich WWU Münster

Introduction to the gradient dynamics description for thin films

We present some the mesoscopic thin-film (or long-wave) hydrodynamic models employed to describe the dynamics of thin films, drops and contact lines of simple liquids on solid substrates. We start with the reformulation of various mesoscopic thin-film hydrodynamic models as gradient dynamics on underlying energy functionals. After briefly presenting the general approach, we discuss deposition patterns in a driven Cahn-Hilliard model for Langmuir-Blodgett transfer of a surfactant layer from the surface of a bath onto a moving plate.

PROGRAM

9.00	A boundary-element approach to dynamic wetting on photo-switchable substrates	**H. Stark**
9.45	Influencing dynamic wetting with polymer brushes and surfactants	**G. K. Auernhammer**
10.30	Coffee	
11.00	Computer simulations of capillary interactions in multiphase flows	**J. Harting**
11.45	The Role of Visco-Elasticity in the Dynamic Wetting of Soft Solids	**S. Karpitschka**
13.00	Lunch	
14.00	Density functional methods for wetting problems	**M. Oettel**
14.45	tba	**D. Helmer**
15.30	Coffee	
16.00	Synthesis and patterning of self-assembled monolayers and polymer brushes	**B. J. Ravoo**
16.45	Wetting and Sorption Properties of Polymer Brushes	**S. de Beer**
17.30	End	

Holger Stark Technische Universität Berlin
and Josua Grawitter

A boundary-element approach to dynamic wetting on photo-switchable substrates

Photo-switchable substrates provide a unique mechanism to manipulate liquid droplets precisely by creating a light-induced wettability landscape, which changes in space and time. Because droplets respond to changes in the wettability of substrates, they can be kept out of equilibrium continuously, giving rise to new states of dynamic wetting. Substrate wettability determines the shape of the droplet contact line and contact angle, i.e., the geometry of its footprint. Changes in droplet shape, in turn, induce droplet motion as well as low-Reynolds number flow inside the droplet. The talk first reviews the basics of hydrodynamics at low Reynolds numbers including the governing Stokes equations. It then introduces the boundary-element method, which we use to determine the dynamics of the droplet shape together with the internal flow field. Here we apply the Navier condition at the interface to the substrate with a non-zero slip length and at the free surface a Neumann condition that links the normal stress component to the curvature, which in hydrostatics is the Laplace pressure. For the contact line we implement the Cox-Voinov law. Finally, we present first results on how droplets respond to a dynamic wettability landscape.

Günther K. Auernhammer IPF Dresden

Influencing dynamic wetting with polymer brushes and surfactants

In this presentation, I will discuss, from an experimental point of view, two ways of influencing dynamic wetting of simple liquids: Adding small amounts of surfactant to the wetting liquid and coating the wetted substrate with polymer brushes. Surfactants change the equilibrium surface tension of aqueous solutions significantly. In wetting and dewetting situations, however, fresh liquid-air interface is been continuously generated at receding contact lines. Since the surface tension of surfactant solutions needs a finite time to reach equilibrium, this generation of fresh surface has important consequences on the dynamics of receding contact lines. This effects can be quantified with detailed measurements of the flow profile close to moving contact lines. Polymer brushes swell when wetted with a solvent. The extend and dynamics of

swelling depends on various parameters like the quality of the solvent. Again, reaching the equilibrium swelling of a polymer brush takes a finite time. So the dynamics of wetting will depend on the relation of the time scales for swelling, deswelling and wetting. In polymer brushes that show special interaction with specific solvents (like co-solvency and co-nonsolvency), this interplay of timescales can be especially rich.

Jens Harting Forschungszentrum Jülich

Computer simulations of capillary interactions in multiphase flows

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 which might be suitable candidates for a new kind of soft, adaptive and switchable substrates.

[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)

Stefan Karpitschka MPI-DS Göttingen

The Role of Visco-Elasticity in the Dynamic Wetting of Soft Solids

The spreading of liquid drops on soft substrates is extremely slow, owing to strong viscoelastic dissipation inside the solid. Despite recent progress, quantitative understanding of the spreading dynamics has remained elusive, partly owing to the difficulty in quantifying the strong viscoelastic deformations be-

low the contact line that determine the shape of moving wetting ridges. In this lecture I will introduce the basic concepts of linear viscoelasticity and demonstrate their use in modeling of moving wetting ridges. I will present direct experimental visualizations of the dynamic wetting ridge shapes, complemented with measurements of the liquid contact angle. It is observed that the wetting ridge exhibits a rotation that follows exactly the liquid angle, as was previously hypothesized [Karpitschka et al., Nat. Commun. (2015)]. This observation is consistent with the model predictions derived in the framework if linear visco- elasto-capillarity. A direct comparison to the theory suggests that moving contact lines lead to a variable surface tension of the soft substrate, following a surface rheology that is distinct from the bulk.

Martin Oettel University of Tübingen

Density functional methods for wetting problems

In this talk I introduce static and dynamic density functional theory (DFT) and discuss its applicability to wetting problems. Illustrations are provided for generic model systems such as simple fluids in the continuum as well a isotropic and anisotropic lattice fluids.

Dorothea Helmer University of Freiburg

tba

tba.

Bart Jan Ravoo WWU Münster

Synthesis and patterning of self-assembled monolayers and polymer brushes

In this tutorial lecture I will introduce the preparation and patterning of self-assembled monolayers and polymer brushes. Self-assembled monolayers are monomolecular films of low molecular weight compounds that adsorb to a suitable substrate. Even if such a monolayer has a thickness of only 1-2 nm, it can completely alter the surface properties of the underlying substrate. Polymer brushes are obtained by grafting-from polymerization of monomers to a surface-immobilized initiator. Depending on the degree of polymerization, the resulting polymer layer can have a thickness from 10-200 nm. The properties of both self-assembled monolayers and polymer brushes can be tuned by the

choice of adsorbate and monomers, respectively. In addition, surface properties can be further engineered by pattering of the layers, e.g. by microcontact printing, nanoimprint lithography or dip pen lithography.

[1] Buten, C.; Lamping, S.; Ravoo, B.J. Acc. Chem. Res. 2019, 52, 1336-1346.
[2] Onclin, S.; Ravoo, B.J.; Reinhoudt, D.N. Angew. Chem. Int. Ed. 2005, 44, 6282-6304.

Sissi de Beer University of Twente

Wetting and Sorption Properties of Polymer Brushes

Decorating surfaces with polymer brushes is an excellent technique to prepare functional designer coatings that can be employed in e.g sensing devices such as electronic noses, separation membranes or moisture harvesting systems. While a lot is known for such brushes under ideal circumstances, it is under investigation how they behave in the complex environments they will be exposed to in applications. In this presentation, I will give an overview of the present state of the art of polymer brush research in the context of wetting and sorption when brushes are exposed to gasses and small droplets.

PROGRAM

9.00	Dynamic Electrowetting at Nanoporous Surfaces: Switchable Spreading, Imbibition, and Elastocapillarity	**P. Huber**
9.45	Understanding processes of wetting and surface patterning in equilibrium and non-equilibrium situations via computer simulations	**A. Heuer**
10.30	Coffee	
11.00	Soft interfaces and their characterization with vibrational sum-frequency generation	**B. Braunschweig**
11.45	Gradient dynamics description for thin films – beyond the single-field case	**U. Thiele**
13.00	Closing and lunch	

Patrick Huber Technische Universität Hamburg

Dynamic Electrowetting at Nanoporous Surfaces: Switchable Spreading, Imbibition, and Elastocapillarity

Electrically conductive substrates, such as surfaces of nanoporous metals and semiconductors allow one to control the wetting energies of electrolytes by electrical potentials. Thereby, it is possible to tune droplet shape and liquid spreading dynamics at surfaces, however also the imbibition into the porous surface is under external control via electrical potential-dependent curvatures of the liquid menisci within the nanopores. Moreover, the enormous Laplace pressures and fluid-solid interfacial stresses, typical of nanopore-confined liquids, induce noticeable deformations of the porous solids, and thus result in the case of electrowetting in a potential-dependent coupling of liquid capillarity to solid elasticity, i.e. electrically switchable elastocapillarity. Starting from planar, unstructured surfaces I will discuss the theoretical backgrounds of these phenomena and relate them to experimental studies on simple aqueous electrolytes at nanoporous solids.

Andreas Heuer WWU Münster

Understanding processes of wetting and surface patterning in equilibrium and non-equilibrium situations via computer simulations

Microscopic computer simulations are of major help to gain a mechanistic understanding of many processes on surfaces. After a short introduction of the simulation methods, including kinetic Monte Carlo, I will address two main topics. (1) In deposition experiments and simulations an additional time scale is given by the deposition rate. We show for serveral examples that a rich phenomenology can be observed when varying that rate. All examples comprise simulation results as well as corresponding experiments. Specific patterns can be obtained when using prepatterned substrates. (2) In wetting of fluids on switchable surfaces (SPP project) first results are presented, dealing with the non-equilibrium properties for the limit of fast switching. Furthermore, we set the path for connecting microscopic and continuum simulations in a multiscale approach.

Björn Braunschweig WWU Münster

Soft interfaces and their characterization with vibrational sum-frequency generation

A molecular understanding of interfaces and their functionalization is of great importance not only from fundamental aspects, but is also highly demanded in specific applications such as functionalization of solid surfaces and the wetting of self-assembled monolayers (SAMs). However, properties like the interfacial molecular structure of a SAM in contact with a liquid as well as the charging state of fluid interfaces are still difficult to address with in situ methods. This is mostly due to a lack of suitable techniques that can interrogate buried surfaces and interfaces on a molecular level. In this respect, vibrational sum-frequency generation (SFG) spectroscopy can be a powerful tool to address hidden interfaces. In this presentation, I will discuss the use of SFG spectroscopy for studies on the molecular self-assembly from a liquid solution to a solid surface and on the wetting as well as dewetting properties of a SAM. For that, results from SFG spectroscopy on the formation, growth and manipulation of phosphonic acid based SAMs on $\alpha - Al_2O_3$ (0001) single crystals, their indentation and the properties of SAMs with new photoswitchable phosphonic acids will be shown and discussed.

Uwe Thiele WWU Münster

Gradient dynamics description for thin films – beyond the single-field case

An overview is given for mesoscopic hydrodynamic (thin-film) models for films and drops beyond the case of a simple liquid on a solid substrate [1,2]. First, we briefly review the concept of gradient dynamics on an underlying free energy for films of volatile simple liquids [2]. Then, cases are considered whose description necessitates (at least) two fields. Particular discussed cases include two-layer films [3], films of mixtures [4] and films/drops covered by insoluble surfactants. Finally, we discuss drops on adaptive substrates [6]. In all cases, we discuss main features of the model and selected physical effects.

[1] U. Thiele, Colloids Surf. A 553, 487-495 (2018).
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[6] U. Thiele, S. Hartmann, http://arxiv.org/abs/1910.10582 (2019).

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THE CENTER FOR NONLINEAR SCIENCE

The study of nonlinear, complex systems is one of the most exciting and fastest growing branches in science nowadays. Understanding the mechanisms governing cooperative, emergent phenomena in complex systems is considered as one of the most important challenges in science, because it is a highly interdisciplinary field that has important applications in fields ranging from physics, mathematics, chemistry, engineering and computer science to life sciences, sociology and finances.

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