

Conference "Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates"

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Book of Abstracts

Keynote talk**Wetting of Polymer surfaces: Effect of Swelling and Droplet Evaporation****Author:** Regine von Klitzing¹¹ *Institute for Condensed Matter Physics, TU Darmstadt*

Wetting of polymer coating is of specific interest for the adhesion of cells or proteins and the technical control of wetting. Cells or proteins are in a physiological environment, i.e. an aqueous solution and the polymer coatings are often hydrophilic or partially hydrophobized. Therefore, the coatings often swell in water which changes the wettability during the wetting process. This complex process is not well understood. A few studies on the water wettability of polyelectrolyte-coated surfaces exist [e.g. 1-4]. Tay et al. found an effect of osmotic pressure on the contact line in wetting studies of charged and uncharged polymeric coatings [5]. That makes the wetting process rather complex, since different time scales but also different length scales come into play. The adaptive surface needs a certain time until the swelling process is finished. The swelling doesn't stop at the three phase contact line, and the liquid sucks laterally into the region in contact with the gas phase. Hansen and Miotto called that it peripheral thickness [6]. This deforms the surface and the contact line is not well-defined anymore.

We studied the wettability by water of polyelectrolyte mono- and multilayers with different polycations or polyanions as the outermost layer using the sessile drop technique [3]. Measurements in a water-saturated atmosphere and in ambient conditions [40% relative humidity (r.h.)] are made to study the effect of swelling and evaporation on the contact angle. It is found that these effects strongly depend on the outermost layer of the polyelectrolyte coating. For several kinds of polyelectrolytes as outermost layer the polyelectrolyte-coated surface can be equilibrated by pre-swelling in saturated vapor. Depositing a water droplet leads to a fixed contact angle against vapor. For other types polyelectrolytes as the outermost layer the water contact angle also indicates a change in the swelling state when the pre-equilibrated film is directly in contact with liquid water, resulting in a decrease in contact angle with time. The studies show that a highly sophisticated interplay between hydrophobic backbone and charge density determines the wetting behavior, irrespective of the sign of surface charge. The stability of the wetting film on polyelectrolyte surface is analysed by disjoining pressure isotherms [7]. There surface charge seems to be the most dominant factor for stability of the wetting film.

[1] Yoo, D., Shiratori, S.S., and Rubner, M.F., *Macromolecules* 1998, 31, 4309.[2] Kolasinska, M. and Warszynski, P. *Bioelectrochemistry* 2005, 66, 65.[3] K. Hänni-Ciunel, G. H. Findenegg, R. v. Klitzing, *Soft Materials* 1998, 5 61.[4] H.-J. Butt, R. Berger, W. Steffen, S. Vollmer, S. A. L. Weber, *Langmuir* 2018 34, 112992.[5] Tay, A., Lequeux, F., Bendejacq, D., Monteux, C., *Soft Matter* 2011, 7, 4715.[6] Hansen, R. S.; Miotto, M., *JACS* 1957, 79, 1765.[7] K. Ciunel, M. Armelin, G. H. Findenegg, R. v. Klitzing, *Langmuir* 2005, 21 4790.**Short talk****Efficient simulation of wetting dynamics on elastic substrates****Authors:** Sebastian Aland¹; Dominic Mokbel¹¹ *TU Freiberg*

The interaction of a viscoelastic substrate with liquid droplets is at small length scales dominated by surface tension forces. Understanding how these forces deform the solid is crucial for the design of new materials, structures, and fabrication techniques.

We present a numerical model to simulate the interaction between two immiscible fluids and an

incompressible viscoelastic solid. The fluid–fluid interface is represented by a phase-field function. The deforming elastic body is described by an additional phase-field [1] or a moving Finite-element grid [2]. Formulating all equations in an Eulerian frame of reference, we obtain a single momentum equation including the solid and both fluid materials.

In numerical tests we demonstrate that this novel method is robust and flexible, and we discuss the advantages and disadvantages of both models ([1] vs. [2]).

[1] Aland, S., Auerbach, P. (2021). A ternary phase-field model for wetting of soft elastic structures. *Int. J. Numer. Meth. Engrg.*, 1–15. <https://doi.org/10.1002/nme.6694>

[2] Aland, S., Mokbel, D. (2021), A unified numerical model for wetting of soft substrates, *International Journal for Numerical Methods in Engineering*, 122, 4, 903-918, <https://doi.org/10.1002/nme.6567>

Short talk

Memory effects of PNiPAAm brushes in different atmospheres

Author: Simon Schubotz¹

Co-authors: Petra Uhlmann¹; Andreas Fery¹; Jens-Uwe Sommer¹; Günter Auernhammer¹

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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 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 seen by consecutively depositing drops at the same position. Previously deposited drops adapt the brush and changes the wetting behavior (advancing contact angle) of subsequent drops [1].

One approach to test for the competition between water and ethanol in the brush, is to measure with a water drop in an ethanol-saturated atmosphere. At the three-phase contact line, the air and probably also the brush will transition from an ethanol-rich state to a water-enriched state. Thus the brush might pass through the regime of the co-nonsolvency effect. On large time scales the ethanol enriched gas phase and the water drop will become mixtures of ethanol and water. We present strategies to counter this mixing effect. The memory effect shown above cannot be experienced in an ethanol-enriched atmosphere.

[1] Schubotz, S., et al., Memory effects in polymer brushes showing co-nonsolvency effects. *Advances in Colloid and Interface Science*, 2021. 294: p. 102442.

Short talk

Lattice Boltzmann simulations of liquid lens coalescence

Author: Thomas Scheel¹

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The lattice Boltzmann method is an efficient approach to simulate complex fluids and wetting processes. We present results based on the colour gradient method which is particularly designed for

multicomponent fluids and is able to obtain thermodynamically consistent results over wide ranges of viscosities and surface tensions. After demonstrating benchmarks to analytically accessible solutions such as the Laplace pressure, Neumann angles, Hagen-Poiseuille velocity profiles or surface tension deduced from drop oscillations, the method is applied to investigate the dynamics of liquid lens coalescence. Thereby the respective asymptotic power-laws obtained from similarity solutions of the thin-film equations are verified in the viscous and inertial limit.

Short talk

Smart surfaces with wetting-programmed topography

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Co-authors: Gissela Constante¹; Indra Apsite¹; Paul Auerbach²; Sebastian Aland²; Dennis Schönfeld³; Thorsten Pretsch³; Pavel Milkin¹

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Living organisms have structured surfaces with specific wettability that allows their efficient adaptation to the environment and improves their survival rate. For example, the rice leaves have micro- and nanoscale structures on their surface that form a superhydrophobic surface for self-cleaning and water repellence [1]. Bioinspiration of these natural surfaces in science can be beneficial for applications in biotechnology, microfluidics, textiles, fabrication of sensors, etc [2]. Addressing these challenging goals requires the development of both materials with tailored properties and methods for the fabrication of structured surfaces. In comparison to previously reported surface patterning techniques, melt-electrowriting is a novel and solvent-free technique that is based on 3D printing and electrospinning which allows programmed deposition of polymeric microfibers [3]. Shape memory polymers offer a very interesting combination of properties such as switching of mechanical properties and capability of stimuli-induced restoration of shape after deformation [4, 5].

This paper reports on fabrication and investigation of wetting properties of structures surfaces with high aspect ratio features (height / width ratio up to 75:1) made using polymers with tunable mechanical properties and shape-memory behavior. It was found that wetting properties of such structured surfaces depend on temperature – surfaces are wetted easier at elevated temperature when polymer is soft because of deformability of lamellae. The deformed morphology can be temporary fixed at low temperature, and it restores to original one by heating above actuation temperature of shape memory polymer. Thus, the high aspect ratio allows tuning of geometry not only manually, as it is done in most works reported previously, but can also be done by placed liquid and is controlled by temperature - a liquid in combination with temperature program topography and wetting properties. This opens new opportunities for design of smart elements of microfluidic devices such as, for example, smart valves.

[1] D.H. Kwon, H.K. Huh, S.J. Lee, *Exp. Fluids* 55(3) (2014) 1691.

[2] Z. Cheng, D. Zhang, X. Luo, H. Lai, Y. Liu, L. Jiang, *Adv. Mater.* 33(6) (2021) 2001718.

[3] P.D. Dalton, *Current Opinion in Biomedical Engineering* 2 (2017) 49-57.

[4] L. Ionov, G. Stoychev, D. Jehnichen, J.U. Sommer, *ACS Applied Materials & Interfaces* 9(5) (2017) 4873-4881.

[5] G. Stoychev, M.J. Razavi, X. Wang, L. Ionov, *Macromol. Rapid Commun.* 38(18) (2017) 1700213.

Short talk

Droplets on substrates with moving and oscillating wettability patterns

Authors: Josua Grawitter¹; Holger Stark¹

¹ *Technische Universität Berlin, Institut für Theoretische Physik*

Droplets are set in motion on substrates with a spatio-temporal wettability pattern as generated, for example, on light-switchable surfaces. To study such cases, we implement the boundary-element method to solve the governing Stokes equations for the fluid flow field inside and on the surface of a droplet and supplement it by the Cox–Voinov law for the dynamics of the contact line. Our approach reproduces the relaxation of an axisymmetric droplet in experiments, which we initiate by instantaneously switching the uniform wettability of a substrate quantified by the equilibrium contact angle.

First, we investigate a droplet on substrates with oscillating uniform wettability by varying minimum and maximum contact angles and frequency. After a transient regime the droplet performs steady oscillations, the amplitude of which decreases with increasing frequency. For slow oscillations our numerical results agree well with the linearized spherical-cap model. They collapse on a master curve when we rescale frequency by a characteristic relaxation time extracted from the spherical cap model. In contrast, for fast oscillations we observe significant deviations from the master curve. Since the droplet's shape changes induce fluid circulation, which is controllable from the outside, our findings envisage the design of targeted microfluidic transport of solutes inside the droplet.

Second, we investigate a droplet on substrates with a moving step profile of wettability, which pushes the droplet towards locations with higher wettability. Using a feedback loop to keep the distance or offset between step and droplet center constant, induces a constant velocity with which the droplet surfs on the wettability step. We analyze the velocity in terms of droplet offset and step width for typical wetting parameters. Moving instead the wettability step with constant speed, we determine the maximally possible droplet velocities under various conditions. The observed droplet speeds agree with the values from the feedback study for the same positive droplet offset. Thus, moving droplets with a wettability step can add to the toolbox of microfluidics.

In the future, we are interested to extend our method to include the effects of substrate adaptivity and to integrate novel findings from experiments in the first phase of the priority program.

Short talk

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

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¹ *Institut für Theoretische Physik, Georg-August Universität Göttingen*

² *Institute of Physical Chemistry, Heidelberg University*

The design of adaptive interlayers between synthetic substrates and soft biological matter is a cross-disciplinary challenge. In analogy to wetting of simple liquids on a solid substrate, one can tailor the adhesion of a cell model (lipid vesicle) by designing the substrate interactions, and the free energy of contact between the substrate and the biological object influences the shape of the vesicle. Similar to the shape of liquid drops on substrates, the shape of a vesicle is dictated by the enclosed volume, the membrane-substrate interactions, and the properties of a lipid bilayer characterized by tension and bending rigidity.

By uniting the experimental and theoretical expertise of our two groups, we investigate the static and dynamic wetting of lipid vesicles on bio-inspired, stimulus-responsive polymer brushes. As the polymer brush systems, we designed bio-inspired polymer brushes that selectively capture divalent heavy metal ions by the multivalent binding to thiol and carboxyl side chains. After confirming the collapse of polymer brushes in the presence of heavy metal ions, the wetting interaction between vesicles and the collapsed/swollen brushes was studied by (i) monitoring the height fluctuation of vesicles using interference contrast microscopy and (ii) analyzing the contact angles using confocal fluorescence microscopy. The change in brush conformation with (collapsed) and without ions (swollen) was utilized to parameterize the non-bonded interactions in the simulation model.

On the theoretical side, we are developing and implementing a numerical model of a vesicle on a

substrate that accounts for the (i) bending rigidity of the lipid membrane, (ii) the interface potential between the solid substrate and membrane, and (iii) the buoyancy of the vesicle. Both, axially symmetric shapes that minimize the free energy as well as fluctuating, triangulated vesicles will be investigated and compared to experiments. Similarities and differences to the wetting of liquid droplets will be highlighted.

Short talk

Drop impact on very thin liquid films on top of hard solid substrates

Author: Kirsten Harth¹

¹ *TH Brandenburg; OVGU Magdeburg*

Drop impact on solid substrates under normal lab conditions typically suffers from effects of substrate inhomogeneities on, e.g., the evolution of interstitial gas films and contact formation. Some recent experiments thus employ micrometer-thin oil films as surficial layers on a hard substrate, but the effect of the film on a droplet's spreading and receding dynamics is typically neglected. However, even few micrometers thin films of viscous fluids do deform. The film's properties influence both contact formation and the receding dynamics of the drop. Actual deformation heights depend on film thickness as well as film properties. The influence of thicker films, or very shallow liquid pools, has become a field of recent interest in the literature. The presentation will address general aspects of droplet dynamics depending on properties of thin spin-coated oil films.

Keynote talk

Energy harvesting due to charge redistribution upon drop impact & Swelling of partly saturated hydrophobic polymer brush layers

Author: Frieder Mugele¹

¹ *Physics of Complex Fluids, University of Twente*

The first part of this lecture I discuss how the energy of falling drops impacting onto pre-charged hydrophobic polymer surfaces can be harvested in an external electrical circuit as screening charges redistribute within the drop.

High speed video imaging and simultaneous electrical measurements lead to a physical model of the energy conversion process including a quantitative analysis of the conversion efficiency [1, 2].

Part two addresses preliminary experiments on the spreading of oil drops with a low vapor pressure on hydrophobic polymer brushes. Within a few hours the swelling process leads to the formation of a pronounced halo around the macroscopic contact line, where the thickness of the partially swollen brush layer varies by a few hundred nanometers over a lateral width of the order of 1mm. The experiments suggest that this seemingly static configuration is in fact stabilized by a very slow gradual evaporation and therefore intrinsically a non-equilibrium phenomenon.

[1] Wu, H., et al., Energy Harvesting from Drops Impacting onto Charged Surfaces. *Physical Review Letters*, 2020. 125: 078301.

[2] Wu, H., et al., Charge Trapping-Based Electricity Generator (CTEG): An Ultrarobust and High Efficiency Nanogenerator for Energy Harvesting from Water Droplets. *Advanced Materials*, 2020. 32: 2001699.

Poster session

HySS – a new wetting regime for on-demand trapping and release of drops

Author: Anil Rajak¹

Co-author: Jürgen Rühle¹

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On hydrophobic rough surfaces, wetting can be described either by Cassie-Baxter model where a drop sits suspended on the structures or by Wenzel model where the drop is penetrated by the structures. The drop in Wenzel regime sticks to the surface which is very difficult to release and in case of Cassie-Baxter regime, the drop is very difficult to trap. We present a new wetting regime, the so-called High Hysteresis Suspended State (HySS) that can be observed on regular patterned micro-trenches. In this regime, the drop suspends like in Cassie-Baxter regime while exhibiting high hysteresis (up to values $>70^\circ$), as in Wenzel state. We present a full model based on our theoretical calculations and experimental results for highly controlled wetting transition between these states (induced by aspect ratio, mass of the drop and applied pressure), trapping of drops and releasing them by an addition of small energy (induced by tilt or mass). With the introduction with HySS, we are also able to demonstrate a dynamic surface for the on-demand tapping and release of drops.

Poster session

Droplets on compressed soft solids

Authors: Hansol Jeon¹; Youchuang Chao¹; Stefan Karpitschka¹

¹ *Max Planck Institute for Dynamics and Self-Organization*

When a liquid droplet rests on a soft surface, capillary forces at the contact line deform the solid into a sharp wetting ridge. The size of the wetting ridge is given by the elasto-capillary length. If the droplet moves, strong viscoelastic dissipation in the soft solid leads to viscoelastic breaking. Recently, it was shown that droplet speeds depend on a pre-stretch of the material, which is incompatible with linear viscoelastic theory. In this poster we discuss visualizations for moving wetting ridges at high spatio-temporal resolution, and recent experiments with droplets on pre-strained materials. Here we apply a compression instead of a stretch and observe a bi-directional interaction of wetting ridges with the creasing instability of compressed surfaces: the deformation under a droplet may trigger creasing, and droplets on creased surfaces move due to the inhomogeneous surface topography. This may have important implications in biology, where materials are typically soft but rarely flat.

Poster session

Rigid and Soft Wetting at Nanoscale

Authors: Nikolai Kubochkin¹; Tatiana Gambaryan-Roisman¹

¹ *Institute for Technical Thermodynamics, Technische Universität Darmstadt*

Wetting phenomena at macro- and microscale have been studied intensively, and significant advancement in the understanding of both statics and dynamics of wetting has been achieved. That resulted in well-established ways to define contact angles and to predict the evolution of the liquid systems. However, due to the current state of imaging techniques, many questions about wetting at the nanoscale and its (dis)similarity to microscaled wetting are left to be unraveled theoretically.

In the present work, we study nanoscaled liquid droplets and rivulets on rigid and soft surfaces. We show that the equilibrium contact angles at the nanoscale depend drastically on the droplet size as well as on the way in which they are defined. Remarkably, the dependencies of the equilibrium contact angle on the droplet height collapse when plotted dimensionless with respect to the range of the surface force action. When the nanodroplet spreads over a wetting film, neither Cox-Voinov nor Tanner laws are valid anymore. Besides, the existence of the wetting film allows capillary ripples to emerge at the advancing front. In contrast to the microscale picture, the ripples are affected by the surface forces and can be fully suppressed by them. Soft substrates respond to the traction exerted by the droplet by forming a wetting ridge. That suppresses the development of the ripples. The wetting ridge height is shown to evolve non-monotonically.

Another focus of the present work is imbibition into corner geometries. It is well known that at macro- and microscale a rivulet must propagate indefinitely along the corner when the sum of half-opening angle of a corner and a contact angle is smaller than ninety degrees. The situation, however, changes when the surface forces are taken into account. Counterintuitively, they stop the rivulet rendering its steady-state even when the condition on spreading described above is fulfilled. We analyze how the corner opening angle, the corner size, and the surface forces influence the static shape of the rivulet. We additionally consider the case when the walls of the corner is soft and, hence, can be deformed by the liquid.

Poster session

Measuring dynamic forces between droplets and polymeric surfaces

Authors: Lukas Hauer¹; Doris Vollmer¹

¹ *Max Planck Institut for Polymer Research*

Droplets sitting on soft, polymeric surfaces form so-called wetting ridges around their three-phase contact line. The vertical component of the droplet's surface tension exerts traction on the surface, leading to elastic deformation of the polymer network and accumulation of unbounded polymer chains. When droplets move over the surface, the wetting ridge moves accordingly, yielding visco- and poroelastic surface responses. The coupling between surface response, free chain reorganization, and the sliding droplet is key to understanding liquid repellency. However, investigations are hampered by the large-scale separation of unbound polymer chains (nanometer), surface (micrometer), and droplet (millimeter). Here, we utilize confocal laser scanning microscopy and interferometry to directly visualize the wetting ridge during droplet motion. Those methods let us distinguish between phases and enable optical resolutions below a micron. A novel optical force sensor let us measure the evolving friction forces between droplets and surface which occur in the order of micro Newton. We show that friction forces scale with velocity and contact lubrication. The presented techniques give new methods to directly determine the coating rheology of soft surfaces.

Poster session

Tuning elastic membrane instabilities for adaptive single and multi-phase fluid transport

Author: Claas-Hendrik Stamp¹

Co-authors: Thomas Pfohl¹; Efsthios Mitropoulos ; Solomon Binyam

¹ *University of Freiburg*

The flexibility and adaptability of microfluidic networks have become more important as the field is rapidly increasing and more sophisticated fluidic systems are going to be introduced in soft autonomous robotics. A new generation of smart fluidic devices requires autonomous feedback-driven

structures which can manipulate droplets, bubbles and fluid flows as well as react to different internal and external stimuli. We are using the coupling of fluid dynamics with newly developed delicate elastic structure designs to manipulate, accelerate and shape single and multiphase flows. The device structures consist of microfluidic networks separated by thin elastic membranes. Local variations of the flow fields, which are controlled by the pressure distribution and the spatial geometric design of the fluidic network, result in spatial-dependent elastic response of the separating membranes, which, in turn, lead to direct feedback on the flow fields. Moreover, using fluid mixtures of solvents with and without membrane swelling capacities, we are not only able to induce membrane instabilities but also to tune the amplitude and wavelength of these instabilities. Surpassing a critical fluid pressure results in an oscillation of the membrane with propagating waveforms. Depending on the fluid pressure as well as on the properties of the membranes, a frequency range of the oscillations from sub Hz to kHz can be covered. This novel microfluidic process design enables us to specifically shape single and multi-phase flows as we introduce a pacemaker or clock into fluidic networks for autonomous smart soft devices.

Poster session

Adaptation of polymer surfaces

Author: Xiaomei Li¹

¹ *Max-Planck-Institut für Polymerforschung*

Polymer surfaces can adapt to liquids in many ways: Liquid can penetrate into polymer layers, polymers can reorient, the liquid induces a chemical reaction and many more [1]. These changes in physical-chemical properties at the interface to the liquid may influence drop shape, velocity, advancing angle and receding contact angle. The aim of our work is to investigate the role of adaptation kinetics for the dynamic contact angles and to compare the results to theory [1]. Therefore, we build up a tilted-plate setup allowing us to measure dynamic contact angles, drop velocity etc. Here, we will discuss results of adaptation processes of a variety of polymer surfaces:

- (a) The adaptation of a random copolymer made from styrene and acrylic acid (PS/PAA) is mainly given by the reorientation of polymer segments at the liquid interface [2, 3].
- (b) The adaptation of the pH-reactive poly (methyl methacrylate-co-8-quinolinyl-sulfide-ethyl acrylate) surface is attributed to the splitting off a hydrophobic group, leading to a more hydrophilic surface. At the same time, the hydrophobic group can act as surfactant for the drop changing the liquid air interface tension. In addition, charge deposition of the sliding drop alters the forces acting on the drop [4].
- (c) The adaptation of poly(N-isopropylacrylamide) (PNIPAM) to water lead to a water tail left behind the sliding drop, which can be caused by polymer reorientation at the interface.
- (d) In the wetting of cross-linked polydimethylsiloxane (PDMS), we observed different modes of wetting: One with a relatively low contact angle hysteresis and one with a larger hysteresis. We conclude that adaptation of the solid-liquid interface is caused by trapped oligomers in the polymer matrix [5].

References:

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- [2] X. Li et al, *Langmuir* 2021, 37, 1571–1577
- [3] X. Li et al, submitted to *Rapid Communications*
- [4] X. Li et al, submitted to *Nature Physics*
- [5] W.S.Y. Wong et al., *Langmuir* 2020, 36, 7236–7245

Poster session

Evaluation of photoswitchable wetting properties of hydrophobic surfaces

Authors: Niloofar Nekoonam¹; Dorothea Helmer¹

¹ *University of Freiburg, Department of Microsystems Engineering*

Spiropyran stands among one of the most interesting molecular switches to induce changes in wetting properties due to the reversible switching between colourless hydrophobic spiropyran to magenta hydrophilic merocyanine by triggers such as light, pH, and metal ions. Spiropyran-induced changes in wetting properties were shown for various purposes and applications, such as antifouling coatings, switchable membranes, and ion sensors (1–4). However, upon any damage or defect to the surface, i.e. to the switchable groups it might lose the switching properties. Therefore, it would be beneficial to have the spiropyran in the bulk of the material, so that spiropyran units are available to show the switch in every layer or region exposed to the trigger. In addition, the wetting properties of the bulk material can be altered upon UV exposure to be used for applications such as membranes (5,6). In this study, two different spiropyran monomers were synthesized (7) and photo-polymerized with other (metha)acrylate monomers to fabricate (non)-porous polymers with switchable wetting properties. Fabricated spiropyran-containing polymeric surfaces showed a micro-meter scale resolution for the switch upon UV exposure using our maskless lithography system (8) and up to 10 ° change in contact angle for smooth surfaces. To enhance the contact angle change, roughness was introduced to the spiropyran-containing polymers by creating porous structures. Our porous photoswitchable polymers containing no fluorinated monomer presented superhydrophobic behaviour (CA > 150°) before and hydrophobic behaviour (CA < 150°) after the switch. The concept will be employed later to achieve switchable wetting properties between superhydrophobic and hydrophilic states.

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Poster session

Lattice models of fluids with Density Functional Theory

Author: Michael Zimmermann¹

Co-author: Martin Oettel ¹

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We use lattice models of particles with hard core repulsion and a short-ranged attraction to describe fluids. Density functionals for such models are introduced and the construction of a dynamic density functional theory is explained.

Previous work in a simple lattice gas model [1] has shown that droplet evaporation and the “coffee ring effect” can be described even though the dynamics neglects hydrodynamic effects. We further discuss improvements and generalizations of the above mentioned model.

[1] Chalmers, C. and Smith, R. and Archer, A.J., Dynamical Density Functional Theory for the Evaporation of Droplets of Nanoparticle Suspension, *Langmuir*, (33,14490–14501),(2017).

Poster session

Swalbe.jl - Droplets, Dewetting, Dynamic Contact Angles

Authors: Stefan Zitz¹; Andrea Scagliarini²; Jens Harting¹

¹ *Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11)*

² *Consiglio Nazionale delle Ricerche, Institute for Applied Mathematics "M. Picone" (IAC)*

Swalbe.jl is an open source lattice Boltzmann based solver for thin film dynamics [1]. Intended for problems ranging from the relaxation or coalescence of droplets to the dewetting of thin films on complex substrates [2]. Features such as thermal fluctuations or spatially resolved contact angles are readily usable and shown to agree with theoretical predictions [3,4]. Switchable substrates can be realized adding a temporal component to the contact angle [5].

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Poster session

Gradient Dynamics Model for Spreading and Coarsening Drops on soft Substrates

Authors: Christopher Henkel¹; Jacco Snoeijer²; Uwe Thiele¹

¹ *WWU Münster*

² *University of Twente*

The investigation of the wetting behavior on viscoelastic or elastic substrates is of great interest. On this poster we present a simple model for liquid drops on fully compressible elastic substrates and show that, besides the doubletransition of steady drops, also dynamic features are captured quantitatively.

In particular we investigate the visco-elastic braking effect, i.e. the increase of dissipation in the substrate with increasing softness, on the example of a spreading drop and show that the scaling laws of a Kelvin-Voigt material [1] are correctly recovered for partially wetting fluids. Beyond that, we explored the coarsening behaviour of two drops and large drop arrays respectively and found that the prevalence of the modes crucially depends on the substrate softness.

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Poster session

Dynamics of liquid droplets on switchable substrates – from microscopic to mesoscopic models

Authors: Leon Topp¹; Moritz Stieneker¹; Andreas Heuer¹; Svetlana Gurevich¹

¹ *WWU Münster*

On this poster we analyse the behavior of a liquid droplet on a switchable substrate theoretically. Therefore we performed molecular dynamics and thin film simulations where we switched the substrate once as well as simulations with periodic switching with different frequencies. Also we developed a mapping between the both models. There we observe different mapping regimes when the surface is switched from a lower to a higher wettability in comparison with the reverse process.

Poster session

Wetting of Photoswitchable Substrates and Polymer Brushes and Their Investigation with Vibrational Sum-Frequency Generation

Authors: Christian Honnigfort¹; Natalia Garcia Rey¹; Björn Braunschweig¹

¹ *WWU Münster*

Smart surfaces that can change their wetting behavior on demand are interesting for applications such as self-cleaning surfaces or tunable lenses. We report on the use of vibrational sum-frequency generation (SFG) to study the molecular structure of photoswitchable surfaces as well as polymer brushes that do show structural adaptation. Results from SFG report on the molecular scale changes and are useful to explain wetting dynamics on macroscopic length scales. In case of polymer brushes, we have addressed the influence of the wetting liquid and the gas phase on the molecular structure of the terminal part of the polymer brush, while for butyl-AAP-C₁₈-PA monolayers we show that E to Z photo switching can trigger a contact angle change by ~10° and that the dynamic changes in contact angle are partially synchronized to the molecular structure changes. For that we have synthesized arylazopyrazole phosphonic acids (butyl-AAP-₁₈-PA) and deposited a monolayer of these molecules on aluminum oxides. The molecular changes were studied by time-resolved vibrational SFG spectroscopy, which provided information on the structural transitions within the AAP monolayer as well as their kinetics. Analysis of SFG spectra has allowed us to determine the characteristic switching times of the monolayer upon irradiation with UV and green light. Further, we demonstrate that interaction of water can stabilize the Z configuration to a large extent. We propose that the exposed polar azo groups of the Z isomer in the AAP monolayer interact strongly with water at the solid-liquid but also at the solid-gas interface, which can stabilize the Z state and hinder the AAP monolayer to switch back into the E state when it is fully immersed in H₂O. Having established the characteristic times for switching on the molecular scale, we have modelled the dynamic contact angle and demonstrate, for the system in our study, that the wetting dynamics are mostly synchronized to the changes on the molecular level.

Poster session

Characteristics of the Dewetting Dynamics and Equilibrium Droplets from Elastic to Visco-Elastic Substrates

Author: Khalil Remini¹

Co-author: Ralf Seemann

¹ *Saarland University*

Dewetting dynamics and the emergence of equilibrium droplet morphologies of polystyrene on top of visco-elastic substrates is considered experimentally. Our initially prepared sample consists typically of glassy polystyrene layer with a molecular weight of 18 kg/mol and a thickness of about 100 nm prepared on top of PDMS viscoelastic substrates. Dewetting is activated by heating the sample above the glass transition temperature of the polystyrene and the dewetting scenario is monitored by atomic force or optical microscopy.

The early stage of the dewetting is characterised by the appearance of holes that increase in diameter with a certain dewetting velocity. Our observations suggest that this dewetting velocity, as well as the morphology of the dewetting rims directly depend in a non-trivial manner on the elastic modulus of the PDMS layer that we vary from 2 MPa to 3 kPa.

When we reach the equilibrium state at the end of the dewetting process, we observe the formation of polystyrene droplets of few microns that could be analysed from both sides (i.e. air/PS and PS/PDMS interfaces) using the lift off technique in combination with atomic force microscopy. Similar to the dewetting dynamics depend the equilibrium droplets shapes on the elastic module of the (visco-)elastic substrates.

In this poster we highlight the major trends and differences that could be observed in our experimental studies, for the dewetting dynamics and equilibrium droplet morphologies with sizes below the elasto-capillary length (i.e. in the limit of a purely viscous substrate), with the idea of extending this study to droplet sizes exceeding the elasto-capillary length (i.e. in the limit of purely elastic substrates)).

Poster session

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

Authors: Marcus Müller¹; Motomu Tanaka²; Lucia Wesenberg¹; Felix Weißenfeld²

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² *Institute of Physical Chemistry, Heidelberg University*

The design of adaptive interlayers between synthetic substrates and soft biological matter is a cross-disciplinary challenge. In analogy to wetting of simple liquids on a solid substrate, one can tailor the adhesion of a cell model (lipid vesicle) by designing the substrate interactions, and the free energy of contact between the substrate and the biological object influences the shape of the vesicle. Similar to the shape of liquid drops on substrates, the shape of a vesicle is dictated by the enclosed volume, the membrane-substrate interactions, and the properties of a lipid bilayer characterized by tension and bending rigidity.

By uniting the experimental and theoretical expertise of our two groups, we investigate the static and dynamic wetting of lipid vesicles on bio-inspired, stimulus-responsive polymer brushes. As the polymer brush systems, we designed bio-inspired polymer brushes that selectively capture divalent heavy metal ions by the multivalent binding to thiol and carboxyl side chains. After confirming the collapse of polymer brushes in the presence of heavy metal ions, the wetting interaction between vesicles and the collapsed/swollen brushes was studied by (i) monitoring the height fluctuation of vesicles using interference contrast microscopy and (ii) analyzing the contact angles using confocal fluorescence microscopy. The change in brush conformation with (collapsed) and without ions (swollen) was utilized to parameterize the non-bonded interactions in the simulation model.

On the theoretical side, we are developing and implementing a numerical model of a vesicle on a substrate that accounts for the (i) bending rigidity of the lipid membrane, (ii) the interface potential between the solid substrate and membrane, and (iii) the buoyancy of the vesicle. Both, axially symmetric shapes that minimize the free energy as well as fluctuating, triangulated vesicles will be investigated and compared to experiments. Similarities and differences to the wetting of liquid droplets will be highlighted.

Keynote talk

Keynote talk

Author: David Quéré¹

¹ *ESPCI Paris; École polytechnique*

(details to be announced)

Short talk

Dynamic Wetting of Self-Assembled Monolayers functionalized with Photoresponsive Arylazopyrazoles

Authors: Niklas Björn Arndt¹; Bart Jan Ravoo¹

Co-author: Friederike Schlüter¹

¹ *WWU Münster*

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 diarylethenes² and spiropyranes³ have been explored in a range of photoresponsive coatings which utilize their photoisomerization to induce changes in macroscopic properties such as wettability.⁴ This results in a substantial and reversible change of wettability.⁵

Current approaches using immobilized photoswitches still suffer from certain drawbacks¹, while in contrast arylazopyrazoles (AAPs) offer significant improvements of photophysical properties. Such as 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 In the talk we present the synthesis of multiple AAP-silane derivatives and the successful functionalization of glass and silicon surfaces using self-assembled monolayers.

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Short talk

Rigid and Soft Wetting at Nanoscale

Authors: Nikolai Kubochkin¹; Tatiana Gambaryan-Roisman¹

¹ *Institute for Technical Thermodynamics, Technische Universität Darmstadt*

Wetting phenomena at macro- and microscale have been studied intensively, and significant advancement in the understanding of both statics and dynamics of wetting has been achieved. That resulted in well-established ways to define contact angles and to predict the evolution of the liquid systems. However, due to the current state of imaging techniques, many questions about wetting at the nanoscale and its (dis)similarity to microscaled wetting are left to be unraveled theoretically.

In the present work, we study nanoscaled liquid droplets and rivulets on rigid and soft surfaces. We show that the equilibrium contact angles at the nanoscale depend drastically on the droplet size as well as on the way in which they are defined. Remarkably, the dependencies of the equilibrium contact angle on the droplet height collapse when plotted dimensionless with respect to the range of the surface force action. When the nanodroplet spreads over a wetting film, neither Cox-Voinov nor Tanner laws are valid anymore. Besides, the existence of the wetting film allows capillary ripples to emerge at the advancing front. In contrast to the microscale picture, the ripples are affected by the surface forces and can be fully suppressed by them. Soft substrates respond to the traction exerted by the droplet by forming a wetting ridge. That suppresses the development of the ripples. The wetting ridge height is shown to evolve non-monotonically.

Another focus of the present work is imbibition into corner geometries. It is well known that at macro- and microscale a rivulet must propagate indefinitely along the corner when the sum of half-opening angle of a corner and a contact angle is smaller than ninety degrees. The situation, however, changes when the surface forces are taken into account. Counterintuitively, they stop the rivulet rendering its steady-state even when the condition on spreading described above is fulfilled. We analyze how the corner opening angle, the corner size, and the surface forces influence the static shape of the rivulet. We additionally consider the case when the walls of the corner is soft and, hence, can be deformed by the liquid.

Short talk

Dynamic wetting phenomena and contact angle hysteresis on polymer brushes and gels

Authors: Lukas Hauer¹; Rodrique Badr²; Doris Vollmer¹; Friederike Schmid²

¹ *Max Planck Institute for Polymer Research*

² *Institut für Physik, Johannes Gutenberg-Universität Mainz*

Droplet mobility on surfaces is achieved by polymeric coatings, in form of gels or brushes, both holding some mobile (free, i.e., un-crosslinked or un-grafted) polymer chains. In the presence of droplets, these free chains accumulate around the three-phase contact line, leading to contact lubrication and wetting ridge formation. The investigation of free chains and understanding their influence on the wetting behaviour is challenging: time and length scales are small (<1 nm, milliseconds) for free chains but huge for droplets (>1 mm, seconds). To bridge the gap between scales, we combine experimental and computational methods and tackle the problem from both ends; Dissipative Particle Dynamics simulations provide insights into the migration of free chains. Confocal laser scanning microscopy and interferometry enable wetting experiments with resolution around 0.1 μm and extensive time resolutions for dynamic measurements. We match simulation and experiments by comparing interfacial energies, wetting ridges, and friction force measurement. The latter is facilitated experimentally by a novel, optical force sensor with a resolution of one micro-Newton. Friction forces can be tuned by droplet speed and surface lubrication (i.e., number of free chains). Finally, we discuss some open questions.

Short talk

Switchable and Adjustable Fluid Transport and Wetting Properties in Polypyrrol-Silicon and Ceramic-based Inverse Opal Structures

Author: Laura Gallardo Domínguez¹

Co-authors: Kaline Furlan ²; Manuel Brinker ³; Patrick Huber ⁴

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Substrates with switchable or adjustable wetting properties are desirable for actuators, coatings, filters or biomedical applications. In this work we present a study of two different substrates. Firstly, the possibilities of an electrically conductive polymer, i.e., polypyrrol in combination with porous silicon are explored, where previous studies already showed how an electric field can influence the chemo-mechanical properties of the polymer [1, 2] and the Young contact angle [3]. Secondly, we analyze the wetting and fluid transport properties of an alumina inverse opal structure (Al₂O₃), which undergoes a spontaneous transition under ambient condition to a more hydrophobic state in time. This transition can be reversed by a low temperature heat treatment. While, a high-temperature heat treatment irreversibly change the porous network structure [4], the low-temperature treatment preserves the inverse opal original structure.

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Short talk

Dynamics of liquid droplets on switchable substrates – from microscopic to mesoscopic models

Authors: Svetlana Gurevich¹; Andreas Heuer¹; Moritz Stieneker¹; Leon Topp¹

¹ *WWU Münster*

In this talk we will theoretically investigate the dynamical properties of a simple liquid on a switchable substrate. To understand the non-equilibrium relaxation dynamics of a liquid droplet on a switchable substrate we study the interplay of different length- and time-scales. We present a method to map the microscopic information, resulting from a molecular dynamics simulation, to a mesoscopic scale, reflected by a thin film model. We analyze the relaxation of a liquid droplet after switching the wettability of the substrate and discuss the cases of the slow and fast periodic switching. Surprisingly, we observe different mapping regimes, depending on the direction of the switching.

Short talk

Dynamic Wetting and Molecular Switching of Photo-Responsive Arylazopyrazole Phosphonic Acid Monolayers on Aluminum Oxide Surfaces

Authors: Christian Honnigfort¹; Natalia Garcia Rey¹; Björn Braunschweig¹

¹ WWU Münster

Smart surfaces that can change their wetting behavior on demand are interesting for applications such as self-cleaning surfaces. In order to functionalize aluminum oxide surfaces, we have synthesized arylazopyrazole phosphonic acids (butyl-AAP-C₁₈PA) that represent a new class of photoswitchable molecules for these oxide surfaces. Butyl-AAP-C₁₈PA monolayers were deposited on α -Al₂O₃(0001) and we show that E to Z photo switching of butyl-AAP-C₁₈PA can trigger a contact angle change by $\sim 10^\circ$. For that we monitored the changes on the macroscopic level by recording the dynamic contact angle, while time-resolved vibrational sum-frequency generation (SFG) spectroscopy provided information on the molecular level as well as on the kinetic changes within the AAP monolayer. Further, we show that a steep decrease in contact angle after initiating E to Z switching with UV irradiation is accompanied by a substantial reduction of the aromatic C-H modes and a non-resonant electronic contribution to the SFG spectra which are both attributable to AAP moieties. In the Z configuration the exposed polar azo groups of the AAP molecules are susceptible to interactions with interfacial water. We show that water can stabilize the Z configuration and hinder the AAP monolayer to switch back into the E state when it is immersed in H₂O, while also water from the gas phase is important for E/Z switching. This is evidenced from substantially different thermal stabilities of the Z configuration in gas phases with different relative humidity. Having established the characteristic times for switching on the molecular scale, we have modelled the dynamic contact angle and demonstrate, for the system in our study, that the wetting dynamics are mostly synchronized to the changes on the molecular level.

Short talk

Droplet motion directed by reversible stiffness gradient on soft switchable surfaces

Authors: Niloofar Nekoonam¹; Dorothea Helmer¹

¹ University of Freiburg, Department of Microsystems Engineering

Liquid droplet manipulation directed by stiffness gradient has been of great interest because of its numerous advantages in applications such as microfluidic systems (1), liquid collection (2), and tissue engineering (3–5). Patterning a stiffness gradient on the surface allows for moving of droplets towards the softer regions or create a well-known durotaxis effect and make them migrate to stiffer regions in a spatially controlled manner. In most systems, the stiffness gradient is patterned permanently and the effect is static so that the droplets move only in certain planned directions. Surfaces with switchable stiffness properties are of high interest to obtain an on-demand and reversible droplet manipulation. In this project, the lecithin-based photorheological fluids (6) based on spiropyran were modified to be employed as a photoswitchable soft surface. In these materials, a stiffness gradient can be created by light at arbitrary regions. Upon UV exposure, the viscosity and stiffness of the surface decrease more than 10- and 3-fold, respectively, which was confirmed by steady-state and dynamic rheological measurements. The properties alteration was due to the UV-induced structural changes of the material because of the photoswitching of spiropyran to merocyanine form. High resolution (7) and reversible stiffness gradient formation on this soft surface using a UV light provided us the opportunity to move the droplet on top of the surface towards softer areas without any stiffness patterning needed in advance. In the future, the concept will be used to manipulate droplets to coalescence and be taken from all over the surface.

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Short talk

Superhydrophobic surfaces using ultra-short pulse structuring of thin metals

Author: Fabian Schäfer¹

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Fabrication of superhydrophobic surfaces induced by ultra-short-pulse lasers is a hotspot of surface studies. We report a way of generating nearly superhydrophobic surfaces on stainless steel (304S15). The method for fabricating this water-repellent surface is to microstructure by irradiating with ultra-short-pulses.

Contact angle measurements were used to investigate the wettability of the surface in relation to the laser parameters (laser fluence and scan line separation). The steady contact angle was investigated in the range of 140°. Investigations with optical measuring methods (white light interferometer) displays the structures of the surfaces. The generated surface shows hierarchical structures with nano and micro roughness similar to a lotus leaf. In further experiments, different materials shall be structured with various structures. Subsequent laser structuring should produce a functional surface with water repellent properties.

Short talk

Liquid Dewetting from Visco-Elastic Substrates

Authors: Khalil Remini¹; Leonie Schmeller²; Ralf Seemann¹; Wagner Barbara²

Co-author: Dirk Peschka²

¹ *Universität des Saarlandes*

² *Weierstrass Institute Berlin*

We investigate the dewetting dynamics and the emerging shape of micron sized liquid polystyrene droplets sitting on a (visco-) elastic substrate with variable E-module spanning from about 2 MPa to 1 kPa using different elastomers.

Experimentally, the droplets are images by atomic force microscopy (AFM) while the deformation of the viscoelastic substrate can be obtained combining AFM with a lift-off technique. The results will be compared to theoretical predictions of a phase-field model that is coupled to finite strain elasticity with a (conserved) Cahn-Hilliard type evolution to understand the interplay of capillary and the nonlinear elastic forces that determine the contact angles and the interfacial morphologies. The numerical algorithm is based on an incremental minimization scheme and equipped with an adaptive mesh and time refinement. This gives a tool to explore different orders of magnitude of the capillary length.

Keynote talk

Elastocapillary Adhesion of Compliant Microspheres

Author: Katharine Jensen¹

¹ *Williams College*

Establishing an adhesive contact between two materials requires both that the surface energies favor the creation of interfacial area and that it is possible to form contact area given the geometry and material properties. While elasticity has long been understood to be important in determining the relative "stickiness" between non-conformal surfaces, in recent years capillarity has also emerged as playing key roles in adhesion with highly compliant materials in multiple ways. For example, recent studies have demonstrated that solid surface tension can compete with or dominate over bulk elasticity in governing contact mechanics on small length scales, and mounting evidence suggests that the internal free fluid phase of compliant polymer gels also contributes significantly to mechanical response via both poroelasticity and classic capillary wetting. In this work, we investigate the adhesion between polydimethylsiloxane (PDMS) gel microspheres and rigid glass substrates. By varying the stiffness and size of the microspheres as well as the surface energy of the substrate and directly imaging the adhered microspheres, we observe a range of adhesive contact geometries from classic elastic to quantitatively wetting-like behavior, always mediated by a phase-separated fluid contact zone. We understand our data with a theoretical model that incorporates elasticity, capillarity, and phase separation to capture the complete range of adhesive contact behavior.

Keynote talk

Dewetting as a probe of properties of polymers at interfaces and in thin films

Author: Günter Reiter¹

¹ *Institute of Physics, University of Freiburg*

The process of dewetting allows to probe the dynamic behavior of polymers within thin films as the response to an applied force, generated directly and intrinsically by interfacial forces and forces acting within the film itself. In addition, taking advantage of the fact that on a single sample the process of dewetting is not initiated everywhere at the same time, one can follow the evolution of a sequence of temporally delayed dewetting processes. Thus, one can examine how nonequilibrium properties of thin polymer films evolve in time. Such sequential dewetting experiments provide a means for determining the time required for equilibration and how viscoelastic properties of the polymer film evolve in time. As one example, the relaxation of residual stresses in thin polymer films can be quantified through the measurement of characteristic parameters of dewetting.

Short talk

Dynamic wetting and dewetting processes on adaptive surfaces

Author: Xiaomei Li¹

¹ *Max-Planck-Institut für Polymerforschung*

When a droplet is sliding on surfaces, adaptation of surfaces leads to changes of the dynamic contact angles [1, 2]. Hereby two adaptation processes play a role: (i) the adaptation of the surface upon

bringing it in contact to the drop (wetting) and (ii) the adaptation of the surface after the drop passed and the surface is in contact with air again (dewetting). In order to study both adaptation processes, we investigated samples made from polystyrene (PS)/polyacrylic acid (PAA) random copolymers by using a tilted-plate method, fluorescence microscope and by sum-frequency generation spectroscopy (SFG) [3]. For the wetting process, the advancing and receding contact angles of water droplets decreased when PS/PAA surface adapted to water. Here, both water diffusion and polymer reorientation play a role in the adaptation process, which were verified by fluorescence microscope measurement and SFG measurement respectively. For subsequent droplets, the sliding velocity decreased which indicates a permanent adaptation. Only by heating the adapted surface over its glass transition temperature (T_g), restored the surface. After this treatment, the droplets reached again the velocity of pristine samples. SFG result indicated that only heating can surface signal recover. Thus, reorientation of the PS-PAA copolymer at the surfaces dominates the dewetting process.

Reference:

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- [2] X. Li et al, *Langmuir* 2021, 37, 1571–1577
- [3] X. Li, M. Encheva et al, submitted to *Macromolecular Rapid Communication* 2021

Short talk

Water Induced Polymer Reorientation at a Polystyrene/Polyacrylic Acid Surface

Authors: Mirela Encheva¹; Xiaomei Li²; Rüdiger Berger²; Ellen H.G. Backus¹

¹ *University of Vienna*

² *Max Planck Institute for Polymer Research*

Certain polymer surfaces undergo an adaptation process after being exposed to liquids due to side chain movements. This reorientation often leads to a preferential exposure of certain polymer groups on the liquid interface, modifying consequently the observed features in surface experiments such as contact angle measurements [1]. This behavior is even more accentuated in block copolymers, where the elements that are most compatible with the liquid are reoriented in order to be in contact with the liquid phase.

In this project, we focus on the adaptation of a random copolymer made out of polystyrene and polyacrylic acid (PS/PAA) upon exposure to water. Previous studies [2] involving contact angle measurements on a tilted plate show a reduction of the contact angle after wetting. Our objective is to determine if this changes in contact angle coincides with a change in surface structure detected by means of sum-frequency generation spectroscopy (SFG).

In our experiments, we evaluated and compared the vibrational SFG spectra of the samples before and after being in contact with water, to determine whether this exposure resulted in a reorientation of the copolymer. In addition, the reversibility of the reorientation by sample annealing over the glass transition temperature (T_g) was also tested.

Due to the intensity change observed in a marker band of the PS polymer in the vibrational SFG spectrum, we were able to confirm a restructuring of the copolymer. Furthermore, we proved that the intensity of this band can be recovered after annealing the samples over the T_g , proving the reversibility of the process [3].

References:

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- [3] X. Li, M. Encheva et al, submitted to *Macromolecular Rapid Communication* 2021.

Short talk

Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows

Author: Dirk Peschka¹

¹ *Weierstrass Institute Berlin*

In this talk, I will present a quick overview of the topics that have been considered in this project

- i. GENERIC Lagrangian-Eulerian formulations of fluid flows,
- ii. Gradient flow descriptions of finite strain elasticity with phase fields,
- iii. Thin-film descriptions with dynamic contact angle,

with a focus on topic iii.

i) The thermodynamic structure of fluid flows in Lagrangian and Eulerian coordinates was investigated, in particular formalizing the reduction framework, cf. Morrison, Marsden, Ratiu, in the GENERIC language. As a result, we obtained an operator framework, that is easily able to generate Poisson and Onsager structures that have been considered in the literature. This is joint work with Marita Thomas and Andrea Zafferi.

ii) Combined finite-strain elasticity and phase fields evolution are modeled as gradient flows and their numerical discretization is considered within the class of incremental minimization schemes. This is joint work with Barbara Wagner, Ralf Seemann, Leonie Schmeller and Khalil Remini.

iii) We consider a variational framework for thin-film flows including dynamic contact angles. In this talk, algorithmic details concerning the higher-order in space and time will be provided and different hierarchies of models will be discussed for gravity-driven sliding droplets and unstable ridges. This is joint work with Luca Heltai, Manuel Gnann, and Lorenzo Giacomelli.

References

* Andrea Zafferi, DP and Marita Thomas (2021) "GENERIC framework for reactive fluid flows" WIAS Preprint (2841). pp. 1-75. ISSN 2198-5855 (Submitted to ZAMM)

* DP and Luca Heltai (2021) "Model hierarchies and higher-order discretisation of time-dependent thin-film free boundary problems with dynamic contact angle" arXiv preprint arXiv:2110.06862. pp. 1-24.

* Leonie Schmeller and DP, "Gradient flows for coupling phase fields and mechanics" (in preparation)

Short talk

Moving wetting ridges: Impact of surface rheology?

Authors: Hansol Jeon¹; Stefan Karpitschka¹

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When a liquid droplet rests on a soft surface, capillary forces at the contact line deform the solid into a sharp wetting ridge. The size of the wetting ridge is given by the elasto-capillary length, but the geometry of the ridge tip is solely governed by the balance of surface tensions. If the droplet moves, strong viscoelastic dissipation in the soft solid leads to viscoelastic breaking. For most soft materials, such as PDMS, dissipation remains integrable, and should thus not impact the tip geometry. Recently, an increase of the ridge opening angle at large speeds was reported, triggering a debate on possible mechanisms. We visualize moving wetting ridges at high spatio-temporal resolution and determine the tip geometry for various liquids and substrate rheologies. We observe an increase of the ridge opening angle at large speeds, even for very mild deformations as caused by the low surface tension of a fluorinated oil. Such phenomenology can be explained by a surface rheology with a relaxation rate that is different from the bulk.

Short talk

Condensing drops on soft substrates

Authors: Ambre Bouillant¹; Martin Essink¹; Christopher Henkel²

¹ *Physics of Fluids, University of Twente*

² *WWU Münster*

The behaviour of drops on rigid and liquid substrates has been investigated extensively in the past and is well understood. However, soft substrates have gained increasing attention recently, since these exhibit elastic properties and can be deformed by liquid on a scale of the elastocapillary length. Soft wetting problems give rise to a wide variety of phenomena that are currently being investigated in many different ways. In this talk we present three such approaches to study condensation on soft solids. Condensation experiments of drops on substrates of different softness has resulted in distinctive breath figures / drop ensembles that indicate softness dependent nucleation probabilities. To better understand these results we employ a simple gradient dynamics model and show that it qualitatively captures the former results. Finally, we used finite element simulations to ensure proper treatment of elasticity and thoroughly investigate the statics of a single drop, particularly focusing on the Shuttleworth effect, i.e. the strain dependence of the solid surface energy.

Short talk

A highly accurate extended discontinuous Galerkin method for multiphase problems with contact lines

Authors: Lauritz Beck¹; Florian Kummer¹

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We present a highly accurate extended discontinuous Galerkin method (XDG) for the simulation of multiphase problems with contact lines. Characteristically, singularities are observed at interfaces and three-phase contact lines between distinct phases, e.g. a jump in pressure or surface tensions. This offers a significant obstacle for high order methods, where generally smooth functions are required to obtain a high order of convergence. By employing a flexible discontinuous polynomial ansatz space, we overcome this restriction and create a method that resolves interface and contact line discontinuities while maintaining a high order of convergence.

We will briefly outline the basic concepts of the XDG method and then concentrate on its central component: interfaces and contact lines. In the XDG method, interfaces are defined implicitly by the zero isocontours of a group of level sets. Each level set describes the interface between two phases, three-phase contact lines are situated at the intersection of two level sets. To elaborate, we will outline algorithms involved in evolving and regularizing the interfaces. Then, we will detail the numerical coupling approach at fluid-fluid and fluid-solid interfaces by means of examples, e.g. the Navier slip boundary conditions on the interface or Neumann's law at the three-phase contact line. We follow the discontinuous Galerkin approach, where terms are linked at boundaries by partial integration and boundary conditions are enforced by penalties. Finally, we will show preliminary results of the simulation of a fluid droplet sitting on a flexible substrate.

Short talk

News from adaptive transport through coupled flow paths

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In our project within the framework of SPP 2171, we are studying and analyzing the transport of fluids and bubbles/droplets in channels interfaced by flexible membranes in microfluidic environments. Our designed microfluidic setup allows for a defined flow-control within the microchannels as well as for the opportunity to analyze fluid transport within the channels and cross-correlations between the channels linked by the elastic membranes. Moreover, initiating and modifying instabilities of the membranes and the feedback in the transport channels, the coupling and cross-communication of the flowing materials and information transport can be amplified and specifically shaped. This membrane-initiated crosstalk will be used to move, adapt, govern, shift and stop specific flows and bubble/droplet motions within fluid transport routes and furthermore to introduce flow patterns with adaption and self-regulation capabilities as well as on the long term logical links and operations within fluid transport networks