

# **SPP 2171 Workshop: "Wetting of Flexible, Adaptive, and Switchable Substrates"**

## **Report of Contributions**

Contribution ID: 2

Type: **Talk**

## An ALE-Phase-Field Method for simulations of wetting on elastic shells in flow

*Wednesday, 7 December 2022 16:30 (30 minutes)*

The dynamics of membranes, shells, and capsules in fluid flow has become an active research area in computational physics and computational biology. The small thickness of these elastic materials enables their efficient approximation as a hypersurface, which exhibits an elastic response to in-plane bending and out-of-plane stretching deformations. If such a closed thin shell is filled with (and/or surrounded by) multiple fluids, capillary forces on the contact line between the fluids and the shell may arise and force the shell to deform.

In this work, we present a novel Arbitrary Lagrangian-Eulerian (ALE) method to simulate such elastic surfaces immersed in Navier-Stokes fluids, which is combined with a phase field approach to model droplets inside and/or outside the surface. This method combines high accuracy with computational efficiency, since the grid is matched to the elastic surface and can therefore be resolved with relatively few grid points near the surface. We formulate elastic surface forces and propose an evolving finite-element discretization. Several wetting test cases demonstrate the versatility of the proposed method. Examples are simulations of single or multiple droplets deforming a vesicle-like shell and approaching different previously defined contact angles.

**Primary authors:** MOKBEL, Marcel (TU Freiberg); ALAND, Sebastian

**Presenter:** MOKBEL, Marcel (TU Freiberg)

**Session Classification:** Short Talks

Contribution ID: 3

Type: **Poster**

## Photoresponsive Wetting of Polymerbrushes containing Arylazopyrazoles

*Monday, 5 December 2022 16:00 (2 hours)*

Arylazopyrazoles (AAPs) are a class of photoswitches and offer significant improvements of more established classes of photoswitches such as azobenzenes. In this work, we present the synthesis of novel poly-thiolactone-hydroxyethyl acrylate-copolymer brushes. These brushes can either be generated to cover a glass or silicon substrate homogeneously or can be structured using microcontact printing ( $\mu$ CP) of the polymerization initiator. Using the unique reactivity of the thiolactones we can introduce photoswitchable AAPs in form of amines as well as linear aliphatic groups in form of acrylates *via* post functionalization. The AAPs enable repeatable photoswitching of the static water contact angle over many cycles while the choice of acrylates can adjust the range of the contact angle change to more hydrophobic or more hydrophilic regions.

**Primary authors:** ARNDT, Niklas Björn; RAVOO, Bart Jan

**Presenter:** ARNDT, Niklas Björn

**Session Classification:** Poster Session

Contribution ID: 4

Type: **Poster**

## The Interplay of Spreading, Imbibition and Evaporation of Droplets at Nanoporous Surfaces

*Monday, 5 December 2022 16:00 (2 hours)*

The dynamics of a droplet deposited on a porous substrate is a combination of three phenomena: spreading, imbibition and evaporation. Here we present a study on the interactions of droplets on nanoporous silicon prepared by electrochemical etching as a function of time. The evolution of the droplet volume is analyzed theoretically and experimentally considering the evaporation and the imbibition of the liquid into the porous substrate. Water is employed to illustrate the case of an evaporation-dominated regime [1]. For an imbibition-dominated regime squalane is employed. The very low vapor pressure of this fluid allows for the analysis of the imbibition process of a droplet into a porous substrate without the contribution of evaporation. The agreement between the experimental data and the theoretical predictions deepens the understanding of the structure of HF-etched porous silicon substrates and provides new insights into the fundamentals of fluid transport in nanoporous media.

**Primary authors:** GALLARDO DOMÍNGUEZ, Laura (TUHH); SANCHEZ, Juan (TUHH); Prof. HUBER, Patrick (TUHH)

**Presenter:** GALLARDO DOMÍNGUEZ, Laura (TUHH)

**Session Classification:** Poster Session

Contribution ID: 5

Type: **Talk**

## Dilute suspensions of chemically active particles in thin liquid films

*Wednesday, 7 December 2022 16:00 (30 minutes)*

Thin liquid films are important for many microfluidic applications such as printing or coating of e.g. printable electronics or photovoltaic cells where an evenly spread thin film of certain properties is of utmost importance as well as so called lab-on-a-chip devices. In biophysics stable thin films play an important role in tear film on eyes or the lining of lungs. On a larger length scale stable thin films are also required in thin-film reactors or even appear in geophysical contexts. It is well known that a thin film on a solid substrate can be unstable and droplet formation may arise, especially for very thin films where gravity cannot dominate surface tension. The dynamics of thin liquid films and their instability has been the subject of intensive experimental, analytical, and numerical studies, the latter often based on the thin film equation. We propose a set of newly developed equations for the influence of chemical active colloids suspended in a thin liquid film based on the lubrication approximation as well as advection-diffusion and the Fick-Jacobs approximation. In order to do so we model the vertical and horizontal distributions of particles within the thin liquid film. We can thereby simplify the problem to a set of three effective parameters. For this novel set of equations we perform a linear stability analysis (LSA) that reveals surprisingly interesting dynamics. We identify the subset of parameters for which the thin film becomes stable i.e. is not rupturing, as well as a variety of different dominating wave-modes. This allows us to control not only the stability but also the droplet form and size distribution after film rupture as well as the time the system takes from a homogeneous to a dewetted state. In order to assess the asymptotic state of the thin film, the LSA results are compared against numerical simulations using the Lattice Boltzmann method. This numerical tool allows us to study the dynamics of such a system more intensely and to evaluate the equilibrium of the system.

**Primary authors:** RICHTER, Tilman (Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien); Dr MALGARETTI, Paolo (Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien); Prof. HARTING, Jens (Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien)

**Presenter:** RICHTER, Tilman (Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien)

**Session Classification:** Short Talks

Contribution ID: 6

Type: **Talk**

## Memory effects of PNiPAAm brushes in different atmospheres

*Thursday, 8 December 2022 11:00 (30 minutes)*

Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. In contrast to previous studies, we concentrate on the partial wetting of co-nonsolvent polymer brushes, i.e., on the dynamics of a three-phase contact line moving over such brushes.

We found that poly(N-isopropylacrylamide) (PNiPAAm) brushes experience a memory effect when consecutively depositing drops at the same position. The subsequent drops adapt the brush and change the drop's wetting behavior (contact angle hysteresis). Hand in hand with the change in the contact angle, hysteresis goes the difference in the force to move the drop laterally. We measure this force with a self-built DAFI.

We measure water drops in an ethanol-saturated atmosphere on PNiPAAm brushes in further wetting experiments. The measurements show that an ethanol-enriched atmosphere strongly affects the memory effect reversibly. At the three-phase contact line, due to the drop's evaporation, the atmosphere's composition and probably the brush will transition from an ethanol-rich state to a water-enriched state. Thus, the brush might pass through the co-nonsolvency regime. 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.

**Primary authors:** SCHUBOTZ, Simon; Prof. SOMMER, Jens-Uwe; Dr UHLMANN, Petra; Prof. FERY, Andreas; Dr AUERNHAMMER, Günter K.

**Presenter:** SCHUBOTZ, Simon

**Session Classification:** Short Talks

Contribution ID: 7

Type: **Poster**

## Stimuli effects on different responsive polymer brushes

*Monday, 5 December 2022 16:00 (2 hours)*

The poly(N-isopropylacrylamide) (PNiPAAm) brush is a very responsive polymer. PNiPAAm reacts to different stimuli like solvent composition, Temperature, and PH. In contrast to previous studies, we vary the chain length and do investigations on PNiPAAm Hydrogels. Furthermore, we compare the PNiPAAm brush to a poly(N-Dimethylacrylamid) (DTMA) brush and argue how the wetting properties change.

Here we investigate how memory effects are affected by different atmospheres. We show how the temperature-induced collapse of the brush changes the wetting properties of the brush. The wetting properties depend not only on the brush but also on their treatment before the heating experiments.

With soft colloidal probe AFM, we investigate the adhesive properties of the brush. We are interested in changes due to co-nonsolvency effects and changes in the adhesive properties due to previous wetting treatment. We compare our findings to lateral force measurements which we perform with a self-built DAFI setup.

**Primary authors:** SCHUBOTZ, Simon; Mr SYCHEV, Dmitrii; Prof. SOMMER, Jens-Uwe; Dr UHLMANN, Petra; Prof. FERY, Andreas; Dr AUERNHAMMER, Günter K.

**Presenter:** SCHUBOTZ, Simon

**Session Classification:** Poster Session

Contribution ID: 8

Type: **Talk**

## Photoswitchable porous substrates for on demand wetting patterns creation

Wednesday, 7 December 2022 14:30 (30 minutes)

Fabrication of smart surfaces with photoswitchable wetting properties is of great interest for applications such as coatings with various wetting patterns[1], sensors[2] or photo-controlled liquid imbibition[3]. Spiropyran stands out among the photoswitchable molecules due to the significant dipole moment change from 4.7 D (SP) to 17.7 D (merocyanine (MC)) featuring a remarkable color change upon UV exposure. However, SP-functionalized surfaces have some drawbacks: any damage or defect to the surface top layer would affect their homogeneous photoswitchable properties, and most fabrication methods such as graft to and graft from are not fully efficient and straightforward.

In this work, synthesized SP monomer was incorporated into the polymeric bulk material, so that the fabricated bulk photoswitchable substrates is still functional after abrasion. A micro/nano-scale roughness was introduced to the surface to amplify the static contact angle (SCA) change by introducing the porosity to the material structure. Polymers with different roughness, i.e. pore size were achieved by varying the porogen content and ratio, and SCA was measured on all the samples before and after UV exposure. In addition, the crosslinker content was found to have an important role to affect the porous structure (roughness) as it implies shrinkage in the pores. According to our results, not only the SP content, but also the pore size, i.e. roughness value is a crucial parameter to tune the photoswitchable wetting properties of the surface. Samples with larger pores, and hence, less SP in contact with the droplet showed insignificant SCA change, while samples with smaller pores could provide SCA changes up to 16.7°. Photo-switched patterns were created on fabricated thin films using a photomask, and on-demand wetting patterns were exhibited. To prove the photoswitchable properties also in the bulk material, thicker samples were cut in half and the SCA change was shown on the cross-section upon UV exposure as well.

### References

- [1] H.S. Lim, J.T. Han, D. Kwak, M. Jin, K. Cho, J. Am. Chem. Soc. 2006, 128, 14458.
- [2] L. Florea, A. Hennart, D. Diamond, F. Benito-Lopez, Sensors and Actuators B: Chemical 2012, 175, 92.
- [3] A. Nayak, H. Liu, G. Belfort, Angew. Chem. 2006, 118, 4200.

**Primary authors:** NEKOONAM, Niloofar; Dr HELMER, Dorothea (Freiburg University, Department of Microsystems Engineering (IMTEK))

**Presenter:** NEKOONAM, Niloofar

**Session Classification:** Short Talks



Contribution ID: 9

Type: **Poster**

## Photoswitchable soft substrates for droplet behavior evaluation upon on-demand softness alteration

*Monday, 5 December 2022 16:00 (2 hours)*

Softness has shown a significant influence on droplet behavior on soft substrates[1]. Alteration of thickness[2], crosslinking degree or curing time[3] on different spots of PDMS or hydrogels[4] have been shown to provide softness patterns which have been used for droplet movement or durotaxis experiments. For further studies and applications, softness patterns that can be switched on-demand on the surface or below the droplet are of high interest. Here, we introduce a photo-switchable gel which shows significant reversible changes in softness upon UV irradiation. The material is based on entangled reverse wormlike micellar systems[5]. These systems are often based on volatile solvents and very low elasticity as their modulus is in the range of a few Pascals. Therefore, we have enhanced the viscoelastic behavior of the material via addition of silica particles, while the photoswitchable properties were preserved. The material was employed as a soft substrate with adjustable softness to evaluate the wetting ridge formation depending on the local softness of a substrate. Wetting ridges were visualized using confocal microscopy on substrates with different silica content, and later compared before and after UV exposure to the substrate. The high resolution of the photoswitchable softness allows softening of one side of the droplet for the investigation of droplet behavior such as asymmetric spreading.

### References

- [1] P.-G. Gennes, F. Brochard-Wyart, D. Quéré, *Capillarity and Wetting Phenomena, Drops, Bubbles, Pearls, Waves*, Springer New York, NY2004.
- [2] R.W. Style, Y. Che, S.J. Park, B.M. Weon, J.H. Je, C. Hyland, G.K. German, M.P. Power, L.A. Wilen, J.S. Wettlaufer, E.R. Dufresne, *Proceedings of the National Academy of Sciences of the United States of America* 2013, 110, 12541.
- [3] S. García, R. Sunyer, A. Olivares, J. Noailly, J. Atencia, X. Trepas, *Lab on a Chip* 2015, 15, 2606.
- [4] I.N. Lee, O. Dobre, D. Richards, C. Ballestrem, J.M. Curran, J.A. Hunt, S.M. Richardson, J. Swift, L.S. Wong, *ACS Applied Materials and Interfaces* 2018, 10, 7765.
- [5] H.-Y. Lee, K.K. Diehn, K. Sun, T. Chen, S.R. Raghavan, *J. Am. Chem. Soc.* 2011, 133, 8461.

**Primary authors:** NEKOONAM, Niloofar; Dr HELMER, Dorothea (Freiburg University, Department of Microsystems Engineering (IMTEK))

**Presenter:** NEKOONAM, Niloofar

**Session Classification:** Poster Session

Contribution ID: 10

Type: **Poster**

## Spreading and Evaporation of Nanodroplets on Soft and Rigid Surfaces

*Monday, 5 December 2022 16:00 (2 hours)*

Droplet spreading and evaporating on complex surfaces is inherent to various natural and industrial processes. While understanding of the wetting dynamics at the macro- and microscale has essentially advanced over the last decades, nanoscale phenomena still leave many questioned unanswered. Since a droplet of a volatile liquid eventually reaches the state when it is comparable to the range of action of the intermolecular (surfaces) forces, it is important to be able to predict its behavior at this evaporation stage.

In the present work, we use a thin-film equation to model the droplet wetting behavior and employ a one-sided kinetically-limited evaporation model. The intermolecular forces are included in the model using the disjoining pressure concept. The case, when a surface in contact with a droplet is soft, is modeled with the help of an analytical solution from a classical theory of elasticity assuming that the surface is a half-space.

We show that droplets evaporate following neither constant contact angle mode nor constant contact radius mode but rather in a mixed mode. Softness of a surface changes the droplet life-time making it shorter, although does not significantly change the general trend followed by the droplet contact angle.

**Primary authors:** KUBOCHKIN, Nikolai (Institute for Technical Thermodynamics, Technische Universität Darmstadt); Prof. GAMBARYAN-ROISMAN, Tatiana (Institute for Technical Thermodynamics, Technische Universität Darmstadt)

**Presenter:** KUBOCHKIN, Nikolai (Institute for Technical Thermodynamics, Technische Universität Darmstadt)

**Session Classification:** Poster Session

Contribution ID: 11

Type: **Poster**

## Dynamic mesoscopic model for two-component compound drops

*Monday, 5 December 2022 16:00 (2 hours)*

We consider a mesoscopic model for two immiscible fluids forming two-layer liquid films or compound drops on a rigid solid substrate. The earlier macroscale description [1,2] is connected to our mesoscopic approach (building on [3]) via consistency conditions. Thereby we relate macroscale and mesoscale versions of the Young and Neumann relations at the liquid 1/ solid/ gas and the liquid 1/ liquid 2/ gas contact lines, respectively. Furthermore, we employ the mesoscale model to investigate selected dewetting and coarsening processes for physically realistic parameters. The steady compound drops emerging from the time simulations are related to bifurcation scenarios determined via macroscale and mesoscale descriptions.

- [1] L. Mahadevan, M. Adda-Bedia, and Y. Pomeau. ``Four-phase merging in sessile compound drops'
- [2] M. J. Neeson et al. \*Compound sessile drops\*. In: *Soft Matter* 8 (2012), pp. 11042\*11050
- [3] A. Pototsky et al. \*Morphology changes in the evolution of liquid two-layer films\*. In:
- [4] Uwe Thiele et al. \*Equilibrium contact angle and adsorption layer properties with surfa

**Primary authors:** DIEKMANN, Jan; Prof. THIELE, Uwe

**Presenter:** DIEKMANN, Jan

**Session Classification:** Poster Session

Contribution ID: 12

Type: Talk

## How friction develops during the sliding of drops

Wednesday, 7 December 2022 15:00 (30 minutes)

Despite many experimental and theoretical studies, it is still impossible to predict dissipative forces, which act against the gravitational forces of drops sliding down an inclined plane. The dissipative forces, which resist drop motion, can be termed “friction force”. In this work, we measured the velocity ( $U$ ), width ( $w$ ), length, advancing contact angle ( $\theta_a$ ), and receding contact angle ( $\theta_r$ ) of liquid drops sliding down inclined flat surfaces. By solving the equation of motion for sliding drops [1], we determined the friction force versus slide velocity for different hydrophobic surfaces. The friction force acting on moving drops of polar and non-polar liquids with viscosities ranging from 0.001 to 1 Pa s can empirically be described by  $F_f(U) = F_0 + \mu w Ca^\alpha$  for the whole relevant velocity range. Here,  $Ca = U\eta/\gamma$  is the capillary number, where  $\eta$  is the viscosity and  $\gamma$  is the surface tension of a liquid. The friction coefficient  $\mu$  is in the range of 1-3 N/m for all liquid/surface combinations. For viscosities  $> 0.006$  Pa s,  $\alpha = 1$ . In these cases, bulk and wedge viscous dissipation fully account for the velocity-dependent friction force. For water and other liquids with  $\eta \leq 0.006$  Pa s, we determined  $\alpha \approx 0.8$ . The latter implies that additional dissipative processes limit drop motion. We confirmed experimental results by numerical diffuse-interface simulations of the flow pattern inside sliding drops. We find that the Furmidge equation [2],  $F = kw\gamma(\cos \theta_r - \cos \theta_a)$ , describes sliding drops as well. The dynamic case, where  $k(U)$ ,  $\mu(U)$ , and  $\alpha(U)$  depend on the slide velocity.  $\mu(U) \approx 1$  is a dimensionless shape factor. For the onset of drop sliding, we determine  $k$  experimentally to be 0.76.

[1] Li, X., Bista, P., Stetten, A.Z. et al. Spontaneous charging affects the motion of sliding drops. *Nat. Phys.* 18, 713–719 (2022). <https://doi.org/10.1038/s41567-022-01563-6>

[2] Furmidge, C. G. L. Studies at Phase Interfaces. I. The Sliding of Liquid Drops on Solid Surfaces and a Theory for Spray Retention. *J. Colloid Sci.* 1962, 17 (4), 309–324.

**Primary authors:** LI, Xiaomei (Max-Planck-Institut für Polymerforschung); Prof. BUTT, Hans-Jürgen Butt (Max Planck Institute for Polymer Research); BODZIONY, Francisco (Computational Multiphase Flows, Technische Universität Darmstadt); Dr MARSCHALL, Holger (Computational Multiphase Flows, Technische Universität Darmstadt); Dr BERGER, Rüdiger (Max Planck Institute for Polymer Research)

**Presenter:** LI, Xiaomei (Max-Planck-Institut für Polymerforschung)

**Session Classification:** Short Talks

Contribution ID: 13

Type: **Poster**

## Schroeder's paradox in polymeric surfaces

*Monday, 5 December 2022 16:00 (2 hours)*

In 1903, von Schroeder reported that gelatin swelled more in water or salt solutions than in the corresponding saturated vapors.[1] Since these phases are in equilibrium, it is surprising that they display different partitioning behaviour, and hence this result has become known as Schroeder's paradox. It has since been found to occur in other cross-linked polymer systems as well, and has received some attention from membrane researchers due to its impact on moisture management in polyelectrolyte membranes. However, its effects on polymeric interfaces, such as gel interfaces or polymer brush coatings, remain relatively unexplored. I present theory and simulations investigating whether Schroeder's paradox occurs in polymer brushes and what its origins may be.

1: Schroeder, P. Über Erstarrungs- und Quellungserscheinungen von Gelatine. Z. Phys. Chem., Stoechiom. Verwandtschaftsl. 1903, 45U, 75, DOI: 10.1515/zpch-1903-4503

**Primary authors:** RITSEMA VAN ECK, Guido (University of Twente); Dr DE BEER, Sissi (University of Twente)

**Presenter:** RITSEMA VAN ECK, Guido (University of Twente)

**Session Classification:** Poster Session

Contribution ID: 14

Type: **Poster**

## Vesicles adhered to flexible and adaptive surfaces

*Monday, 5 December 2022 16:00 (2 hours)*

Vesicles play a fundamental role in many biological processes, such as the transport of neurotransmitters between synapses. Another example, involving much larger vesicles, is trees, where vesicle-surface interaction is implicated in regulating their nutrient intake. During these processes, the adhesion behavior of vesicles to soft biological surfaces is crucial. Consequently, it is important to understand the factors, which determine whether a vesicle adheres and what shape it will adopt in contact with a flexible and adaptive surface.

Here, we systematically study the adhesion of a vesicle to planar, undeformable surfaces, vesicles, and droplets of various sizes. We assume an axially symmetric system with finite-range interactions throughout our simulations. Previous studies often considered a contact potential of zero range. However, as synaptic vesicles ( $d \sim 40\text{nm}$ ) are relatively small, the effect of the potential range has to be considered. The contact of the vesicle is characterized by the balance between bending and adhesion energy, which scale differently with the vesicle size. Additionally, in the case of vesicle-vesicle or vesicle-droplet contact, the size ratio is of importance as is the ratio between the bending rigidity and bending rigidity/rescaled intrinsic surface tension. The interplay of these different characteristics gives rise to a complex diagram of shapes.

**Primary authors:** WESENBERG, Lucia; Prof. MÜLLER, Marcus (Uni Göttingen)

**Presenter:** WESENBERG, Lucia

**Session Classification:** Poster Session

Contribution ID: 15

Type: **Talk**

## Cloaking Induced Variation in Droplet Surface Tension

*Thursday, 8 December 2022 09:45 (45 minutes)*

Cloaking of surface material (e.g. oligomers in PDMS coatings) on contacting droplets is a phenomenon that directly affects static and dynamic wetting. Of the multitude of changes that the system undergoes with cloaking, the change in the effective droplet surface tension is the most conspicuous. The small length scale of the cloak (in the order of nanometers) together with the imposed curvature of the droplet surface makes direct experimental monitoring (static and dynamic) challenging. Here, we tackle this problem with a combination of MD simulations and surface tension measurements. The former resolves locally the degree of the cloak while the latter resolves the temporal evolution of the cloak using the surface tension as a proxy. The analysis is finally supplemented with a theoretical framework, motivated by the results.

**Primary authors:** Mr BADR, Rodrique (JGU Mainz); Mr HAUER, Lukas (MPIP Mainz); Prof. VOLLMER, Doris (MPIP Mainz); Prof. SCHMID, Friederike (JGU Mainz)

**Presenters:** Mr BADR, Rodrique (JGU Mainz); Mr HAUER, Lukas (MPIP Mainz)

Contribution ID: 16

Type: **Talk**

## **Influence of surface chemistry on the charging of water drops moving on hydrophobic silicate substrates**

*Tuesday, 6 December 2022 12:00 (30 minutes)*

In the last few years a lot of studies have shown that by contact/slide electrification between water droplets and hydrophobic surfaces, it is possible to generate electricity in an environmentally friendly way. In the first applications LEDs could operate in this way[1] The physical processes are still being discussed today. To extend the understanding Stetten et al.[2] have established an experimental setup that allows to study the drop charge of individual drops. In the work presented here we have studied with this setup the influence of the surface chemistry to the charge of moving water droplets at hydrophobic silicate substrates. We were able to show here that the chemistry of the substrate plays a central role and that the origin of the charge of the droplets is caused by hydration of the surface.

References:

[1] C. Wu, A. C. Wang, W. Ding, H. Guo, Z. L. Wang, *Advanced Energy Materials* 2019, 9, 1802906.

[2] A. Z. Stetten, D. S. Golovko, S. A. Weber, H.-J. Butt, *Soft Matter* 2019, 15, 8667-8679.

**Primary authors:** Mr LEIBAUER, Benjamin; Prof. STEFFEN, Werner; Prof. BUTT, Hans-Jürgen

**Presenter:** Mr LEIBAUER, Benjamin

**Session Classification:** Short Talks



Contribution ID: 17

Type: **Poster**

## Synthesis of diblock copolymer brush surfaces to control the adaptation time to water

*Monday, 5 December 2022 16:00 (2 hours)*

Young model describes the wetting behavior of an ideal surface. Recently, Butt et al., presented a model which connects adaptation processes of the surface to dynamic contact angles.[1] In the first phase of the SPP project, we developed an experimental setup which allows measuring adaptation processes. Li et al., used random copolymer surfaces to confirm the adaptation model.[2] Now, in the second phase of the SPP project, we want to synthesize polymer surfaces where we can control the adaptation time scale upon wetting and dewetting systematically. For this purpose, we use the Atom Transfer Radical Polymerization (ATRP) to selectively synthesize copolymer brushes consisting of a hydrophilic and hydrophobic block. In our synthesis we immobilized an ATRP initiator on a silicon wafer. Then we prepared PHEMA (Poly-2-hydroxyethyl methacrylate) as hydrophilic block from the initiated surface. In the next step we grafted Polystyrene or PEHMA (2-ethylhexyl methacrylate) as hydrophobic block from the first polymer block as a (macro)initiator. We realized grafted blockcopolymer brush films with a systematic variation of the molecular weights of PHEMA, PS and PEHMA. First results showed that with a layer of 13 nm PS brushes grafted from PHEMA (16 nm) the water contact angle (CA) is the same as on a pure PS surface (advancing contact angle= $93\pm 2^\circ$ ; RCA= $94\pm 3^\circ$ ).

### References:

- [1]: Butt, H.J.; Berger R. et al.; Adaptive Wetting-Adaptation in Wetting, Langmuir 2018, 34 (38), 11292-11304  
[2]: Li X.; Berger R. et al.; Adaptation of a styrene-acrylic acid copolymer surface to water, Langmuir 37, 1571-1577 (2021)

**Primary authors:** Mr LEIBAUER, Benjamin; Dr DE LOS SANTOS PEREIRA, Andres; Dr POP-GEORGIEVSKI, Ognen; Prof. BUTT, Hans-Jürgen; Dr BERGER, Rüdiger

**Presenter:** Mr LEIBAUER, Benjamin

**Session Classification:** Poster Session

Contribution ID: 18

Type: **Talk**

## A High-Order Method for the Interaction of Fluids and Soft Substrates with Three-Phase Contact Lines

*Tuesday, 6 December 2022 14:00 (30 minutes)*

We present a highly accurate extended discontinuous Galerkin method (XDG) for the simulation of multiphase problems involving three-phase contact lines on a flexible solid. We will show results of a simulation of a water droplet sitting on a silicone-gel, utilizing Navier slip boundary conditions on the interface and Young's equation at the three-phase contact line. Characteristically, singularities are observed at interfaces and three-phase contact lines between distinct phases, e.g. a jump in pressure or surface tensions. This is problematic for high order methods, where generally smooth functions are required to obtain 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 [1]. 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 and we will detail the numerical coupling approach at fluid-fluid and fluid-solid interfaces by means of examples.

### REFERENCES:

- [1] Kummer, F., 2017. Extended discontinuous Galerkin methods for two-phase flows: the spatial discretization. *Int. J. Numer. Meth. Engng*, 109: 259– 289.
- [2] Wang, Y. and Oberlack, M. A thermodynamic model of multiphase flows with moving interfaces and contact line. *Continuum Mechanics and Thermodynamics* (2011) 23, Article Number: 409.

**Primary authors:** KUMMER, Florian (TU Darmstadt - FG Strömungsdynamik); BECK, Lauritz (TU Darmstadt - FG Strömungsdynamik)

**Presenter:** KUMMER, Florian (TU Darmstadt - FG Strömungsdynamik)

**Session Classification:** Short Talks

Contribution ID: 19

Type: **Talk**

## Steering droplets on substrates with plane-wave wettability patterns and deformations

*Wednesday, 7 December 2022 17:00 (30 minutes)*

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 Cox–Voinov friction for the dynamics of the contact line. One objective of our research is targeted microfluidic transport of such droplets. In earlier work we investigated how a droplet can be steered by controlling its substrate’s wettability pattern [Grawitter and Stark, *Soft Matter* **17**, 2454 (2021)]. As a next step, we have recently extended our method to include substrates the height profile of which varies temporally in a prescribed manner.

We compare two cases: First, we investigate a droplet on substrates with planar-wave-like wettability profile by varying the speed and wave length of the pattern. Second, we investigate a droplet on substrates which deform periodically according to a planar-wave profile. In both scenarios, when the profile moves slowly, it moves the droplet moves steadily forward. Above a critical pattern speed the droplet performs steady oscillations. These speed oscillations correspond to oscillations in the shape of the droplet which decay linearly as a functions of pattern speed.

**Primary authors:** GRAWITTER, Josua (Technische Universität Berlin, Institut für Theoretische Physik); Prof. STARK, Holger (Technische Universität Berlin, Insitut für Theoretische Physik)

**Presenter:** GRAWITTER, Josua (Technische Universität Berlin, Institut für Theoretische Physik)

**Session Classification:** Short Talks

Contribution ID: 20

Type: **Talk**

## Describing liquid drops on elastic substrates: Mesoscale model vs. macroscale model and experiment

*Tuesday, 6 December 2022 11:30 (30 minutes)*

We investigate the behaviour of liquid drops on soft viscoelastic substrates employing mesoscopic and macroscopic models as well as experiments.

First we introduce a simple mesoscopic gradient dynamics model and show that it recovers the known double-transition in contact angles with

increasing softness and that it is well suited to study multi-drop problems like the dependence of drop coarsening on softness [1]. Second, we incorporate the Shuttleworth effect and compare the mesoscopic results with a macroscopic neo-Hookean model with proper treatment of bulk elasticity in a large-deformation framework [2]. Finally, we present experiments showing that condensation of drops on substrates of different softness results in distinctive breath figures / drop ensembles that indicate softness dependent nucleation probabilities. Extending the mesoscopic model to incorporate condensation allows us to predict the dependence of nucleation probability on softness and compare

it with experimental results.

[1] Henkel C., Snoeijer J. H., Thiele U. 2021 Gradient-dynamics model for liquid drops on elastic substrates. *Soft Matter* 17, 10359–10375, DOI: 10.1039/d1sm01032h

[2] Henkel C., Essink M. H., Hoang T., van Zwieten G. J., van Brummelen E. H., Thiele U., Snoeijer J. H. 2022 Soft wetting with (a)symmetric Shuttleworth effect. *Proc. R. Soc. A* 478: 20220132. DOI: 10.1098/rspa.2022.0132

**Primary authors:** HENKEL, Christopher (Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany); ESSINK, Martin H. (Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands); BUIILLANT, Ambre (Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands); Prof. THIELE, Uwe (Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany); Prof. SNOEIJER, Jacco H. (Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands)

**Presenters:** HENKEL, Christopher (Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany); ESSINK, Martin H. (Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands)

**Session Classification:** Short Talks

Contribution ID: 21

Type: **Poster**

## Gradient Dynamics Model for Liquid Drops on Elastic Substrates - Capturing prominent Soft Wetting Phenomena using a simplified Approach

*Monday, 5 December 2022 16:00 (2 hours)*

We investigate the behaviour of liquid drops on elastic substrates employing a simplified formulation of elasticity corresponding to the Winkler foundation model. By using a gradient dynamics approach we obtained a versatile and numerically less expensive model allowing for the treatment of statics and dynamics of both single drops as well as large drop ensembles. While a previous version has been used to qualitatively recover basic phenomena of soft wetting, like the double transition of contact angles and viscoelastic breaking [1], we recently extended the model to incorporate horizontal displacement as well as surface elasticity. In the course of that the impact of the Shuttleworth effect has been studied for different symmetry scenarios and compared to a macroscopic neo-Hookean model with proper treatment of bulk elasticity in a large-deformation framework [2].

[1] Henkel C., Snoeijer J. H., Thiele U. 2021 Gradient-dynamics model for liquid drops on elastic substrates. *Soft Matter* 17, 10359–10375, DOI: 10.1039/d1sm01032h

[2] Henkel C., Essink M. H., Hoang T., van Zwieten G. J., van Brummelen E. H., Thiele U., Snoeijer J. H. 2022 Soft wetting with (a)symmetric Shuttleworth effect. *Proc. R. Soc. A* 478: 20220132. DOI: 10.1098/rspa.2022.0132

**Primary authors:** HENKEL, Christopher; ESSINK, Martin H. (Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands); Prof. SNOEIJER, Jacco H. (Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands); Prof. THIELE, Uwe (Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany)

**Presenter:** HENKEL, Christopher

**Session Classification:** Poster Session

Contribution ID: 22

Type: **Talk**

## Monitoring of Water Penetration in Polymer Brushes by Time-Resolved Fluorescence of Solvatochromic Dye

*Tuesday, 6 December 2022 11:00 (30 minutes)*

The (de)wetting of e.g. polymer-coated surfaces with various liquids is of fundamental importance in equilibrium and molecular dynamics in confined mesoscale media and is also vital in many materials and applications. In particular, the response of switchable polymer layers to an externally applied thermal, optical, electrical or chemical stimulus causes alternation of local properties, in particular local polarity and molecular mobility. To model such switching, two factors are of crucial importance: (1) the relaxation rate and (2) the width of the contact region, which influences the apparent contact angle for water drop on the surface. Because of the experimental limitations, however, fast subsecond relaxation processes, which may be involved in the dynamic wetting, have been hitherto not addressed for fluorescence imaging.

In the second phase of this SPP we plan to visualize this by analyzing the time-resolved fluorescence of novel polarity sensitive solvatochromic dyes. In this contribution we introduce the overall project idea and discuss our preliminary work with the well-known dye Nile red (NR). The absorption and fluorescence spectra of NR are significantly shifted to the red when solvent polarity increases. In addition, the fluorescence lifetime increases in polar solvents and decreases in protic solvents. These two measurable quantities allow one to image the spatial xyz-distribution of media polarity as well as protic solvent (water) content in different transient states of polymer layers during (de)wetting with water.

In order to overcome the  $\mu\text{m}$ -limited optical z-resolution in the nanoscale layers, specially designed depth-gradient dye-labelled polymer brushes will be prepared. There the growing grafted from the surface polymer chain will be labelled with the reporter dye at different nanoscale depth (z). The depth will be gradually changed with respect to the macroscale lateral axis (x). In this experiment the fluorescence color image and/or fluorescence lifetime images (FLIM) of the polymer layer map the liquid diffusion in the layer as well as polymer reorganization during (de)wetting process in the front and in the tail of droplets moving along the x-direction.

Our preliminary data, which shows that this idea is feasible, are based on thermally-switchable poly(di(ethylene glycol) methyl ether methacrylate) (PDEGMA) polymer brush layers that were grown from glass surfaces. From the fluorescence spectra of NR loaded via simple partitioning without control of z in the PDEGMA brushes, the polarity of the polymer is estimated to be between that of ethyl acetate and acetone. PDEGMA also shows a LCST behavior. It is hydrated below 32°C and collapses above this temperature. The fluorescence of NR in PDEGMA brushes decays double exponentially with major long-lived (4.6 ns) and minor short-lived (2.1 ns) components. When the temperature varies from 20 to 50 °C, strong deswelling of PDEGMA (swelling ratio from 3 at 25 to 1.5 at 50 °C) is accompanied with a substantial reduction (from 0.22 to 0.12) of the contribution of NR short-lived decay component. The random distribution of NR in the brushes does not allow one to map these observables in a depth resolved manner. This is overcome in the SPP project by gradient brushes.

**Primary author:** Dr DRUZHININ, Sergey I. (Physical Chemistry I, Department of Chemistry and

Biology and Research Center of Micro and Nanochemistry and (Bio)Technology (C $\mu$ ), University of Siegen)

**Co-authors:** Mr GREITER, Michael (Physical Chemistry I, Department of Chemistry and Biology and Research Center of Micro and Nanochemistry and (Bio)Technology (C $\mu$ ), University of Siegen); Prof. IHMELS, Heiko (Organic Chemistry II Department of Chemistry and Biology and Research Center of Micro and Nanochemistry and (Bio)Technology (C $\mu$ ), University of Siegen); Prof. SCHÖNHERR, Holger (Physical Chemistry I, Department of Chemistry and Biology, University of Siegen and Research Center of Micro and Nanochemistry and (Bio)Technology (C $\mu$ ), University of Siegen)

**Presenter:** Dr DRUZHININ, Sergey I. (Physical Chemistry I, Department of Chemistry and Biology and Research Center of Micro and Nanochemistry and (Bio)Technology (C $\mu$ ), University of Siegen)

**Session Classification:** Short Talks

Contribution ID: 23

Type: **Poster**

## Spreading of volatile oils on swelling hydrophobic polymer brush layers

*Monday, 5 December 2022 16:00 (2 hours)*

Polymer brushes are highly responsive materials that have a broad spectrum of possible applications, therefore an understanding of their interfacial behavior is essential. The degree of swelling of a polymer brush can be influenced by various external stimuli, such as the presence of a solvent. Under good solvent conditions, drop spreading causes changes in the wettability of the brush surface resulting in a finite contact angle. We observe this in a system of hydrophobic poly lauryl methacrylate (PLMA) solvated by a droplet of hexadecane. A halo is visible ahead of the slowly advancing contact line resulting from a gradient in degree of swelling. The width of the halo is the result of a complex coupling of solvent transport between the brush, droplet, and vapor. The time-dependent swelling profile in the halo region is modelled by numerical calculations using gradient dynamics, as extracted from interferometry measurements. Experiments with solvents with various vapor pressures (variable alkane chain length) are performed to further understand the spreading dynamics of a drop on complex surfaces and reveal the mechanism of the halo formation and the wetting phenomena.

**Primary author:** Mr REUVEKAMP, Sander (University of Twente, SPC group)

**Co-authors:** Dr KAP, Özlem (University of Twente, PCF group); Mr HOEK, Harmen (University of Twente, PCF group); Mr SIEKMAN, Vincent (University of Twente, PCF group); Dr DE BEER, Sissi (University of Twente); Dr SIRETANU, Igor (University of Twente, PCF group); Prof. MUGELE, Frieder (University of Twente, PCF group)

**Presenters:** Mr REUVEKAMP, Sander (University of Twente, SPC group); Mr SIEKMAN, Vincent (University of Twente, PCF group)

**Session Classification:** Poster Session



Contribution ID: 24

Type: **Poster**

## Fluorescent Techniques to Measure in Real-Time Water Diffusion Through Polymeric Surfaces

*Monday, 5 December 2022 16:00 (2 hours)*

Fluorescent dyes are widely used in fluorescence microscopy, providing important advantages such as the detection of specific components or changes in the surrounding medium of a component of interest. The variety of commercial fluorescent dyes and their stability make these tools ideal for potential implementation as probes of molecular-scale changes. In particular, we are interested in implementing different fluorescent dyes for the real-time measurement of droplet diffusion through polymeric surfaces and their participation in the adaptation of the structure of these polymeric structures when they are in contact with water.

Our current set-up contemplates the use of a monolayer of pHrodo Green dye sensitive to changes in pH adhered to a glass cover slip and the subsequent deposition of a layer of Polyacrylic Acid (hydrophilic) on which a drop of solution of Ph 4. Using a confocal fluorescence microscope, the change in the intensity of the fluorescent light was measured in real time before and during the deposition of the droplet to find time constants that allow us to analyze the adaptation and interaction of the polymeric surface in contact with the drop.

**Primary author:** CATALÁN, Karina (Sandoval)

**Presenter:** CATALÁN, Karina (Sandoval)

**Session Classification:** Poster Session

Contribution ID: 25

Type: **Poster**

## Sliding water contact electrification on plasma-treated surface

*Monday, 5 December 2022 16:00 (2 hours)*

Water drops moving down inclined hydrophobic and insulating surfaces acquire a charge and deposit counter charges onto the solid surface. This charge separation by sliding drops is also called slide electrification. One of the general observations on fluorinated polymers is that sliding drops leave negative charges on surfaces. Our aim here is to determine if charging processes can be controlled by already existing charges at surfaces deposited by other means. How do these changes influence the potential of sliding drops and the charge that is carried away. This understanding will then be useful for understanding of surfaces with different wetting properties. To clean surfaces, often plasma treatment is involved as an essential step. Here we address the question of how plasma treatment influences the charging of Fluorinated SU-8 surface and sliding water drops. While fluorinated SU-8 shows the normal drop charge-versus-drop number (Q-vs-n) behaviour, the curve for plasma-treated surfaces is very different. Surface charge was examined by Kelvin probe and zeta potential.

**Primary authors:** Ms DARVISH, Fahimeh (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Dr BERGER, Rüdiger (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Prof. STEFFEN, Werner (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Prof. BUTT, Hans-Jürgen (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany)

**Presenter:** Ms DARVISH, Fahimeh (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany)

**Session Classification:** Poster Session

Contribution ID: 26

Type: **Poster**

## Deep learning to analyze sliding drops

*Monday, 5 December 2022 16:00 (2 hours)*

State-of-the-art contact angle measurements usually involve image analysis of sessile drops. The drops are symmetric and images can be taken at high-resolution. The analysis of videos of drops sliding down a tilted plate is hampered due to the low-resolution of the cutout area where the drop is visible. The challenge is to analyze all video images automatically, while the drops are not symmetric anymore and contact angles change while sliding down the tilted plate. To increase the accuracy of contact angles, we present a 4-segment super-resolution optimized-fitting (4S-SROF) method. We developed a deep learning based super-resolution model with an up-scale ratio of 3; i.e. the trained model is able to enlarge drop images 9 times accurately (PSNR=34.9). In addition, a systematic experiment using synthetic images was conducted to determine the best parameters for polynomial fitting of contact angles. Our method improved the accuracy by 21% for contact angles lower than 90° and by 33% for contact angles higher than 90°.

**Primary authors:** Mr SHUMALY, Sajjad (Max Planck institute for polymer research); Ms DARVISH, Fahimeh (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Ms LI, Xiaomei (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Mr SAAL, Alexander (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Mr HINDUJA, Chirag (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Prof. STEFFEN, Werner (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Dr KUKHARENKO, Oleksandra (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Prof. BUTT, Hans-Jürgen (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); Dr BERGER, Rüdiger (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany)

**Presenter:** Mr SHUMALY, Sajjad (Max Planck institute for polymer research)

**Session Classification:** Poster Session

Contribution ID: 27

Type: **Keynote**

## Solid-liquid work of adhesion

*Monday, 5 December 2022 14:45 (45 minutes)*

We discuss the problem of solid liquid adhesion and in particular we will focus on a tool for direct measurements of the work needed to separate a liquid from a solid. The method mimics a pendant drop that is subjected to a gravitational force that is slowly increasing until the solid-liquid contact area starts to shrink spontaneously. The work of adhesion is then calculated in analogy to Tate's law. The values obtained are intensive (independent of drop size) and in agreement with Dupré's theory.

**Primary author:** Prof. TADMOR, Rafael

**Presenter:** Prof. TADMOR, Rafael

Contribution ID: 28

Type: **Keynote**

## Lift at low Reynolds number

*Wednesday, 7 December 2022 09:00 (45 minutes)*

Soft and wet contact arises in a range of phenomena that spans many length and time scales, and includes: landslides, aquaplaning of tires, wear of industrial bearings, ageing of synovial and cartilaginous joints, cell motion in blood vessels or microfluidic devices, and atomic-force or surface-force rheology. Therein, the coupling between boundary elasticity and confined viscous flow leads to a striking zoology of counterintuitive emergent effects. From the canonical situation of a free particle that can simultaneously sediment, slide, and roll in a viscous fluid, and near a soft wall, we study a range of novel inertial-like (despite the low-Reynolds-number flow) features, such as: enhanced sedimentation, elastohydrodynamic bouncing, roll reversal, emergent lift and torque, dynamical adhesive-like forces.

**Primary author:** SALEZ, Thomas (LOMA @ CNRS & Univ. Bordeaux)

**Presenter:** SALEZ, Thomas (LOMA @ CNRS & Univ. Bordeaux)

Contribution ID: 30

Type: **Keynote**

## Wetting and Swelling of soft fibres

*Thursday, 8 December 2022 09:00 (45 minutes)*

We consider the morphologies adopted by liquid in fibrous assemblies, and in particular the coupled effects of geometry, elasticity and swelling on the liquid distribution. For favorable solvents that are absorbed by the fibers, the induced swelling strongly affects the liquid distribution, for example inducing transient motions or even coalescence of the drops. When the fibers are flexible, the force exerted by the drop may deform them. Swelling can induce a spontaneous collapse of the fibers and a forced imbibition, which we rationalize with a model coupling poroelasticity and elasto-capillarity.

**Primary author:** DUPRAT, Camille (Ecole Polytechnique)

**Presenter:** DUPRAT, Camille (Ecole Polytechnique)

Contribution ID: 32

Type: **Talk**

## Equilibrium droplets between experiment and theoretical predictions

*Wednesday, 7 December 2022 14:00 (30 minutes)*

In this study we are interested in Polystyrene liquid droplets in equilibrium on PDMS elastic solid substrates in the limit of the electrocapillary length, and consequently to the ratio between the surface tensions and the elasticity of the substrates. An experimental analysis using Atomic Force Microscopy of the different parameters constituting the shape of micron-sized droplets in both the free interface and the interface in contact with the PDMS (obtained using a lift-off technique) are compared to our theoretical model where we establish a general framework for coupling phase fields to mechanics in form of a gradient-flow structure. This leads to a thermodynamically consistent model that allows for different types of coupling and dissipation mechanisms. For this, we construct robust numerical algorithms based on an incremental minimization scheme. We can then use this tool to investigate different orders of magnitude of capillary length

**Primary authors:** REMINI, Khalil (Saarland University); SCHMELLER, Leonie

**Presenters:** REMINI, Khalil (Saarland University); SCHMELLER, Leonie

**Session Classification:** Short Talks

Contribution ID: 33

Type: **Talk**

## High voltages generated by sliding drops

Slide electrification is a spontaneous charge separation between a substrate and a sliding drop. Here, we describe this effect in terms of a voltage generated at the three-phase contact line. This voltage is on the order of 0.2-2 kV and moves charges between the drop and the substrate. We model this system by a surface- and drop capacitor connected to the voltage source of the moving three-phase contact line. To model previous drop charge experiments and experiments on more exotic substrates with drop-rate dependent charge polarity, we introduced an adaptation of the contact-line voltage upon water contact. Using this adaptive two capacitor model, we can describe a wide range of experiments, enabling new insights into the molecular details of the charge separation mechanism.

**Primary authors:** Mr BISTA, Pravash (MPI for Polymer Research); Dr STETTEN, Amy (MPI for Polymer Research); Dr WONG, William (MPI for Polymer Research); Prof. BUTT, Hans-Jürgen (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); WEBER, Stefan (MPI for Polymer Research Mainz)

**Presenter:** WEBER, Stefan (MPI for Polymer Research Mainz)

**Session Classification:** Short Talks



Contribution ID: 34

Type: **Talk**

## Fast contact line on soft solids

*Tuesday, 6 December 2022 15:00 (30 minutes)*

When a droplet is resting on a soft surface, the capillary forces deform the surface into a sharp wetting ridge. The amplitude of the wetting ridge is determined by elasto-capillary length, but the angles by which the interfaces meet at the ridge tip only depend on the balance of surface tensions, the so-called Neumann balance. For moving contact lines, dissipation in the wetting ridge leads to viscoelastic braking. In recent literature, various effects that could alter Neumann balance and viscoelastic braking have been suggested: free, extractable oligomers, strain-dependent solid surface tension, or point forces emerging from bulk viscoelasticity.

We visualize moving wetting ridges at high spatio-temporal resolution and determine the tip geometry for various liquids and PDMS substrates. With these different materials, we tune, on the one hand, the elasto-capillary length over a wide range that allows us to resolve the near field of the ridge tip, orders of magnitude below the elasto-capillary length. On the other hand, we tune the ratio of liquid and solid surface tensions, going from the much-studied, highly non-linear regime (e.g. water on PDMS) to a regime where the Neumann balance and linear viscoelasticity theory may be used.

We experimentally resolve the logarithmic curvature singularity of the ridge near its tip, caused by the singular traction of the contact line, to a degree that allows a faithful determination of the solid angles. These differ significantly from the prediction obtained by Neumann's law and the surface tensions against non-crosslinked PDMS, pointing to a strain-dependent solid surface tension. We further show that dissipation remains regular for moving wetting ridges. However, we also show that dissipation is more localized than linear theory predicts, even for mild solid opening angles.

**Primary author:** JEON, Hansol (Max Planck Institute for Dynamics and Self-Organization)

**Co-author:** Dr KARPITSCHKA, Stefan (Max Planck Institute for Dynamics and Self-Organization)

**Presenter:** JEON, Hansol (Max Planck Institute for Dynamics and Self-Organization)

**Session Classification:** Short Talks

Contribution ID: 35

Type: **Keynote**

## **Charging and adaptation after wetting**

*Monday, 5 December 2022 14:00 (45 minutes)*

tba.

**Primary author:** BUTT, Hans-Jürgen (Max Planck Institute for Polymer Research)

**Presenter:** BUTT, Hans-Jürgen (Max Planck Institute for Polymer Research)

Contribution ID: 36

Type: **Talk**

## Gradient dynamics model for sessile drop evaporation in a gap: from simple to applied scenarios

*Thursday, 8 December 2022 12:00 (30 minutes)*

We consider an evaporating drop of volatile partially wetting liquid on a rigid solid substrate. In addition, the setup is covered with a plate, forming a narrow gap with the substrate. First, we develop an efficient mesoscopic description of the liquid and vapor dynamics in a gradient dynamics form.

It couples the diffusive dynamics of the vertically averaged vapour density in the narrow gap to an evolution equation for the drop profile.

The dynamics is purely driven by a free energy functional that incorporates wetting, bulk and interface energies of the liquid as well as vapour entropy.

Subsequently, we employ numerical simulations to validate the model against both experiments and simulations based on Stokes equation.

Finally, we show that the gradient dynamics approach allows for extensions of our model to cover more intricate scenarios, e.g., spreading drops of volatile liquid on polymer brushes or on porous media.

**Primary authors:** HARTMANN, Simon; THIELE, Uwe (WWU Münster); DIDDENS, Christian (University of Twente); JALAAL, Mazyar (University of Amsterdam)

**Presenter:** HARTMANN, Simon

**Session Classification:** Short Talks

Contribution ID: 38

Type: **Keynote**

# Stimulus-Induced Wetting of Polymer Brushes with Lipid Vesicles: Experimental Challenges and Perspectives

*Wednesday, 7 December 2022 11:00 (45 minutes)*

Adhesion of biological cells and lipid vesicles shares common features with wetting droplets. The main difference from the droplets of simple liquid is that the deformation is not only driven by tension but also by bending elasticity of membranes. Inspired by proteins, we designed polymer brushes that switch the conformation by complexation with heavy metal ions. The switching of thickness, density and interfacial roughness was detected by high energy X-ray reflectivity, and the switching of interfacial viscoelasticity was monitored under systematic variation of heavy metal ion concentrations. The detailed shape and height fluctuation of vesicles were determined by microinterferometry, while the global shape of vesicle was reconstructed from confocal images. From the height fluctuation of the bottom surface of vesicles, we determined the critical threshold that induces a transition from “non-wetting” to “wetting”, and the precise shape analysis near the contact line yielded the free energy of adhesion. Recently, we successfully observed the “dynamic” switching of wetting vesicles in a microfluidic chamber, which opens a possibility to investigate the kinetics of switchable wetting with lipid vesicles.

**Primary author:** TANAKA, Motomu (Ruprecht-Karls-Universität Heidelberg)

**Presenter:** TANAKA, Motomu (Ruprecht-Karls-Universität Heidelberg)

Contribution ID: 39

Type: **Talk**

## Molecular Kinetics and Dynamic Wetting of Self-Assembled Monolayers with Arylazopyrazole Photoswitches on Oxide Surfaces

*Tuesday, 6 December 2022 14:30 (30 minutes)*

In this presentation we report on self-assembled monolayers (SAMs) with photo-switchable arylazopyrazole (AAP) silanes [1] on SiO<sub>2</sub> surfaces as well as AAP phosphonic acids [2] on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> which exhibit fluorinated and aliphatic terminal groups, respectively. By switching the AAP moiety in the SAM from their E to their Z state, the molecules are driven from a linear to a bend configuration which exposes the more hydrophilic azo group. This causes changes in surface wettability and a change in static contact angle of about 10°. We have now analysed the molecular kinetics of the photoswitchable SAMs in detail using both vibrational sum-frequency generation (SFG) and dynamic contact angle measurements. For that, we have systematically changed the surface coverage of the AAP photoswitches by changing either the deposition time of the fluorinated AAP or by adjusting the Langmuir-Blodgett transfer of the AAP phosphonic acids to the aluminium oxide substrates. Previously, we have shown that the drop and substrate dynamics are coupled and that using an analytical model one can determine the molecular kinetics of the AAP during dynamic wetting [2]. In fact, the kinetics of the wetted monolayer are surprisingly slow, which we have now addressed on a molecular level by using surfaces of different coverage. This has allowed us to discuss the role of packing density of the SAMs on the dynamic wetting of the monolayer.

[1] N. Arndt, F. Schlüter, M. Böckmann, T. Adolphs, H. F. Arlinghaus, N. L. Doltsinis, and B. J. Ravoo, *Langmuir* **38**, 735-742 (2022)

[2] H. Honnigfort, L. Topp, N. García Rey, A. Heuer, B. Braunschweig, Dynamic Wetting of Photo-Responsive Arylazopyrazole Monolayers is Controlled by the Molecular Kinetics of the Monolayer, *J. Am. Chem. Soc.* **144**, 4026-4038 (2022)

**Primary authors:** Ms GOLOMB, Melanie (WWU Münster); ARNDT, Niklas Björn; HONNIGFORT, Christian; RAVOO, Bart Jan; BRAUNSCHEWIG, Björn

**Presenter:** BRAUNSCHEWIG, Björn

**Session Classification:** Short Talks

Contribution ID: 40

Type: **Talk**

## Water droplets on liquid crystal-infused porous surfaces

*Wednesday, 7 December 2022 11:45 (30 minutes)*

The design of open surface microfluidics that enables orthogonal control of liquid mobility and chemical composition is crucial for devising the next generation of microfluidic platforms that will find use in applications across chemical, environmental, and biomedical fields. To achieve these functionalities, extensive studies have demonstrated stimuli-responsive liquid mobility on open platforms based on either micro/nanoscale topographical surfaces or water-immiscible liquid-coated surfaces. However, methods of manipulating droplets' chemical compositions tend to rely upon chemical adsorption directly from the underlying surface, which has been shown to subsequently pin droplets to the surface and render them immobile.

We report the design of a liquid crystal (LC)-based open surface microfluidic platform that enables the independent manipulation of the mobility and chemical compositions of droplets. Specifically, we use porous LC polymeric networks to stabilize thermotropic LC mesogens to overcome the issue of water-induced LC dewetting. We find that the mobility of water droplets on LC-based surfaces depends on the positional order of the LC. Moreover, we experimentally demonstrate that the mesogenic orientational order of the LC surface plays a pivotal role in the release of chemicals from the LC surface to droplets. Finally, we investigate the effect of water droplet impact behaviors (bouncing, spreading, retraction, wetting) on such surfaces. We primarily focus on the deposition regime where surface chemistry, roughness, and wettability of the LC mesophase play an important role in the early stage of the post-impact dynamics.

**Primary author:** Dr TKALEC, Uroš (University of Ljubljana)

**Co-authors:** Mr ŠTANC, Rok (University of Ljubljana); Prof. WANG, Xiaoguang (Ohio State University)

**Presenter:** Dr TKALEC, Uroš (University of Ljubljana)

**Session Classification:** Short Talks

Contribution ID: 41

Type: **Keynote**

## Solvation and Wetting of Polymer Brushes in Air

*Tuesday, 6 December 2022 09:00 (45 minutes)*

For the development of brush-based functional surface-coatings, it is critical to understand their properties, because they will determine their performance and user-experience. Polymer brush solvation and wetting are key parameters in this. In this presentation we will show that brushes can display counter-intuitive wetting properties. We aim to unravel those by combining molecular dynamics simulations, contact angle goniometry and ellipsometry laboratory experiments.

**Primary author:** DE BEER, Sissi (University of Twente)

**Presenter:** DE BEER, Sissi (University of Twente)

Contribution ID: 42

Type: **Talk**

## Dip-coating a soft layer

*Thursday, 8 December 2022 11:30 (30 minutes)*

A solid, withdrawn from a wetting liquid bath, entrains a thin liquid film. This simple process, first described by Landau, Levich, and Derjaguin (LLD), is commonly observed in everyday life. It also plays a central role in liquid capture by animals, and is widely used for surface-coating purposes in industry. Motivated by the emerging interest in the mechanics of very soft materials, and in particular the resulting elastocapillary coupling, we develop a dip-coating model that accounts for the additional presence of a soft solid layer atop the rigid plate. The elastic response of this soft layer is described by a Winkler's foundation. Using a combination of numerical, scaling, and asymptotic-matching methods, we find a new softness-dependent power-law regime for the thickness of entrained liquid at a small capillary number, which corresponds to a modified physics at play in the dynamic meniscus. The crossover between this regime and the classical dip-coating one occurs when the substrate's deformation is comparable to the thickness of the entrained liquid film.

**Primary authors:** BERTIN, Vincent (University of Twente); Prof. SNOEIJER, Jacco H. (Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands); Prof. RAPHAEL, Elie (ESPCI Paris); SALEZ, Thomas (LOMA @ CNRS & Univ. Bordeaux)

**Presenter:** BERTIN, Vincent (University of Twente)

**Session Classification:** Short Talks



Contribution ID: 43

Type: **Keynote**

## Switchable and Adaptive Bioadhesion - Insights from Living Systems

*Tuesday, 6 December 2022 09:45 (45 minutes)*

Among all living species, microbes are the most abundant and diverse form of life on Earth. They have conquered almost all ecosystems of our planet by successfully adapting to their environment. Life on Earth has evolved under the exposure of sunlight and many species are equipped with a photosynthesis machinery enabling them to transform light into chemical energy. Their microhabitats include liquid-infused soil, porous rocks and microdroplets, featuring complex geometric architectures that support strong spatial and temporal fluctuations of light exposure. Thus, developing functionalities to rapidly respond to light fluctuations, far more than other environmental cues, has been pivotal for natural selection.

In this presentation, I will show how experimental methods from soft matter physics and biophysics [1], in conjunction with theoretical concepts from non-equilibrium statistical physics, enable us to decipher fundamental physical principles of the light response of photosynthetic microorganisms. In particular, I will focus on the interactions of light-sensing microbes with abiotic surfaces [2] and discuss in detail, how the bioadhesion of living microbes can be highly adaptive [3,4] and even reversibly switchable within seconds [5].

[1] M. Backholm and O. Bäumchen, *Nature Protocols* 14, 594 (2019); [2] S. Till et al., *Physical Review Research*, accepted (2022); [3] C.T. Kreis et al., *Soft Matter* 15, 3027 (2019); [4] N. Xu et al., *eLife* 9, e58805 (2020); [5] C.T. Kreis et al., *Nature Physics* 14, 45 (2018).

**Primary author:** BÄUMCHEN, Oliver (University of Bayreuth)

**Presenter:** BÄUMCHEN, Oliver (University of Bayreuth)

Contribution ID: 44

Type: **not specified**

## **Climate crisis: Impressions from the UN Climate Change Conference, COP 27. Our role as scientists.**

*Tuesday, 6 December 2022 16:00 (1 hour)*

Evening talk: report from the recent climate conference COP27.

**Primary author:** VOLLMER, Doris (Max Planck Institute for Polymer Research)

**Presenter:** VOLLMER, Doris (Max Planck Institute for Polymer Research)

Contribution ID: 45

Type: **Keynote**

## Biological Applications of the Thin-Film-Equation: From cellular motility to lateral spreading of biofilms

*Wednesday, 7 December 2022 09:45 (45 minutes)*

In biological systems activity can manifest itself in different forms; as individual motility or as growth and production processes. I will present two different applications of the thin film equation coupled to active processes.

In both scenarios, the (reductionist's) model equations represent a gradient dynamics derived from a potential energy supplemented by bioactive terms which break the symmetry of the gradient dynamics.

In the first scenario, I introduce a model for individual cell motility driven by active stress. Eukaryotic cells may translocate on homogeneous substrates by employing their cytoskeleton, an assembly of polar filaments and molecular motors.

I will discuss this model within the context of bistability observed in keratocytes, which may coexist as immotile and motile cells.

In the second scenario, I will introduce a model for lateral biofilm spreading. When encountering surfaces or interfaces, many bacteria transition from a planktonic to a community lifestyle. The thereby formed bacterial colonies grow by cell division and spread as flat films along the interface. Here I will highlight the importance of passive surface forces and osmotic fluxes, compared to individual bacterial motility, for biofilm spreading on agar substrates under air.

**Primary author:** JOHN, Karin (Université Grenoble-Alpes, CNRS, LIPhy, 38000 Grenoble, France)

**Co-authors:** STEGEMERTEN, Fenna (WWU Münster); TRINSCHEK, Sarah (FH Münster University of Applied Sciences); LECUYER, Sigolène (Université Lyon, ENS de Lyon, Université Claude Bernard, CNRS, Laboratoire de Physique, 69342 Lyon, France)

**Presenter:** JOHN, Karin (Université Grenoble-Alpes, CNRS, LIPhy, 38000 Grenoble, France)

Contribution ID: 47

Type: **Talk**

## **Bistable moving and resting drops in an active thin-film model**

*Wednesday, 7 December 2022 12:15 (30 minutes)*

We present a simple model, derived from basic thermodynamic principles, for active polar free-surface droplets to identify a mechanism of motility in the context of cell crawling. Namely, active stresses drive drop motion through spatial variations of polarization strength. This robustly induces parity-symmetry breaking and motility even for liquid ridges (2D drops) and adds to splay- and bend-driven pumping in 3D geometries. Intriguingly, then, stable polar moving and axisymmetric resting states are bistable, reminiscent of the interconversion of moving and resting keratocytes by external stimuli. The identified additional motility mode originates from a competition between the elastic bulk energy and the polarity control exerted by the drop surface. As it already breaks parity-symmetry for passive drops, the resulting back-forth asymmetry enables active stresses to effectively pump liquid and drop motion ensues.

**Primary author:** STEGEMERTEN, Fenna (WWU Münster)

**Presenter:** STEGEMERTEN, Fenna (WWU Münster)

**Session Classification:** Short Talks

Contribution ID: 48

Type: **Poster**

## Intelligent Polymer Materials and Films for Electrochemical, Pharmaceutical & Soft Robotics Applications

*Monday, 5 December 2022 16:00 (2 hours)*

This poster will give insights into current research activities of the Ludwigs team. In our interdisciplinary and international research team of polymer chemists, physical chemists and materials scientists we are developing functional and intelligent polymer materials and devices for electrochemical, pharmaceutical and soft robotics applications. One of our aims is to control and manipulate structure-function relationships of hierarchical architectures from the molecular via the nanoscopic to the macroscopic scale such as block copolymer self-assembly and controlled crystallization of semicrystalline polymers.

Going beyond structure-function relationships stimuli-responsive polymers have come in the interest of our research, because their properties show a response when triggered by external environmental conditions such as change in relative humidity, temperature or electric fields, exhibiting great potential for the development of smart devices.

Conjugated (e.g. polythiophenes) and redox polymer (e.g. carbazole-bearing polymer) films are studied in terms of their electrochemical doping behavior [1,2] and with respect to electrochemical switching and doping between different redox states, e.g. for electrochromism or pore control in block copolymer templates.

In a recent paper, the mechanical properties of bilayer actuators as a function of relative humidity were examined in detail in collaboration with the group of Prof. Holger Steeb. By fabricating a bilayer out of a hydrophobic and a hydrophilic polymer (PDMS and PEDOT:PSS, respectively), our group managed to create a humidity-triggered actuator. Due to the fact that the mechanical properties of PEDOT:PSS depend strongly on the relative humidity (r.H.), it was possible to predict the curvature of the humidity-triggered bilayer actuators by the humidity-dependence of the mechanical properties. [3]

### References

- (1) D. Neusser, C. Malacrida, M. Kern, Y. Gross, J. van Slageren, S. Ludwigs, *Chem. Mater.*, 2020, 32, 6003.
- (2) C. Malacrida, Y. Lu, K. Dirnberger, S. Gámez-Valenzuela, M. C. Ruiz Delgado, S. Ludwigs, *J. Mater. Chem. C* 2020, Doi: <https://doi.org/10.1039/D0TC03090B>.
- (3) C. Dingler, H. Müller, M. Wieland, D. Fauser, H. Steeb, S. Ludwigs, *Adv. Mater.*, 2021, 33, 2007982.

**Primary author:** LU, Junqi (University of Stuttgart)

**Co-author:** LUDWIGS, Sabine (University of Stuttgart)

**Presenter:** LU, Junqi (University of Stuttgart)

**Session Classification:** Poster Session