

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

## **Reporte der Beiträge**

Beitrag ID: 1

Typ: **Poster**

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

Montag, 4. Dezember 2023 18:10 (20 Minuten)

Synthesis of diblock copolymer brush layers to control the adaptation time to water

Benjamin Leibauer<sup>1</sup>, Andres de los Santos Pereira<sup>2</sup>, Sajjad Shumaly<sup>1</sup>, Ognen Pop-Georgievski<sup>2</sup>, Hans-Jürgen Butt<sup>1</sup>, Rüdiger Berger<sup>1</sup>

<sup>1</sup> Departement Physics at Interfaces –Max Planck Institute for Polymer Research

<sup>2</sup> Institute of Macromolecular Chemistry CAS, Prague

Abstract, SPP 2171 Meeting Berlin, December 2023

The Young's model describes the wetting behavior of an ideal surface. Recently, Butt et al. presented an adaptation model, which connects adaptation processes of the surface to dynamic contact angles [1]. In order to test the adaptation model, we used a tilted plate setup, which allows measuring velocity dependent contact angles. The applicability of the adaptation model was experimentally verified by Li et al. using surfaces made of statistical copolymers [2,3]. The adaptation model was used to measure the release kinetics of a pH-responsive polymer [4]. In a next step, we synthesize polymer surfaces with the aim to control the adaptation time scale upon wetting and dewetting systematically. We used the surface-initiated atom transfer radical polymerization ATRP to selectively synthesize diblock copolymer brushes. We prepared poly(2-hydroxyethyl methacrylate) (PHEMA) as a hydrophilic block from the surface and we grafted polystyrene (PS) or Poly(1-hexyl methacrylate) (PEtHexMA) as hydrophobic block on top of the PHEMA block [5]. By regulating the architecture and thickness of the polymer brush we tune the wetting properties. In addition, we control the adaptation time of polymer brush surfaces by changing the drop-sample temperature.

References

[1] Hans-Jürgen Butt, Rüdiger Berger, Werner Steffen, Doris Vollmer, and Stefan A. L. Weber, *Langmuir*, 34, 11292 - 11304 (2018). [10.1021/acs.langmuir.8b01783](https://doi.org/10.1021/acs.langmuir.8b01783) ...

[2] Xiaomei Li, Simon Silge, Alexander Saal, Gunnar Kircher, Kaloian Koynov, Rüdiger Berger, Hans-Jürgen Butt, *Langmuir* 37, 1571-1577 (2021). <https://doi.org/10.1021/acs.langmuir.0c03226> ...

[3] Xiaomei Li, Mirela Encheva, Hans-Jürgen Butt, Ellen H.G. Backus and Rüdiger Berger, *Macromol. Rapid Commun.* 43, 2100733 (2022). <https://doi.org/10.1002/marc.202100733>

[4] Xiaomei Li, Krisada Auepattana-Aumrung, Hans-Jürgen Butt, Daniel Crespy, Rüdiger Berger, *Chemical Physics Letters* 158, 144901 (2023). <https://doi.org/10.1063/5.0142928>

[5] Benjamin Leibauer, Andres de los Santos Pereira, Ognen Pop-Georgievski, Hans-Jürgen Butt, Rüdiger Berger manuscript in preparation

*emphasized text*

**Hauptautoren:** LEIBAUER, Benjamin; Dr. DE LOS SANTOS PEREIRA, Andres (Institute of Macromolecular Chemistry CAS, Prague); Dr. BERGER, Rüdiger (MPIP); Herr SHUMALY, Sajjad; Dr. POP-GEORGIEVSKI, Ognen (Institute of Macromolecular Chemistry CAS, Prague); Prof. BUTT, Hans-Jürgen (MPIP)

**Vortragende(r):** LEIBAUER, Benjamin

**Sitzung Einordnung:** Poster Session

Beitrag ID: 2

Typ: **Poster**

## Estimating the drop width based on side view dynamic measures

Montag, 4. Dezember 2023 16:30 (20 Minuten)

The analysis of sliding drop videos have emerged as a valuable tool for investigating physical phenomena (1-3). Hereby, automatic image processing enables the extraction of various measures from these videos (4, 5). On homogeneous surfaces, hydrodynamic dissipation increases with velocity. Recently, Li et al. studied drops sliding down an inclined surfaces (3) and reported an empirical equation that describes the velocity-dependent friction force:

$$F_f = F_0 + \beta w U \eta \quad (1)$$

Where,  $F_0$  is the friction force extrapolated to velocity  $U = 0$ ,  $\beta$  is a dimensionless friction coefficient,  $w$  is the width of the droplet while sliding, and  $\eta$  is the viscosity of the liquid. The geometry of drops and their kinetic contact angles sliding down an inclined plane change with velocity. These parameters can be readily measured in side view. However, monitoring drop width in sliding drop experiments typically requires additional equipment such as a camera or mirrors, which limit the effective sliding length in videos from 5 cm to 1.5 cm. Therefore, the slide length can only be investigated partially and sections of the slide length might be missed where defects on the surface are present. A method to estimating the drop width based on side view dynamic measures is required.

We investigated the use of different regression and multiple multivariate sequence analysis (MMSA) models to estimate drop width based solely on side view measures. Our results demonstrated that temporal dependencies play a crucial role in this use case, with the LSTM model outperforming the other models tested. The LSTM model achieved a best result of 67  $\mu\text{m}$  based on root mean square error (RMSE), whereas the regression model achieved a best result of 109  $\mu\text{m}$ . When taking into account the full range of actual drop width values, an RMSE of 67  $\mu\text{m}$  translates to an error rate of roughly 5%. This finding suggests that the LSTM model is a promising approach for accurately estimating drop width in sliding drop videos without requiring additional equipment. In particular, the LSTM model enables accurate estimation of drop width for the entire 5 cm sliding length.

References:

1. Li X, Bista P, Stetten AZ, Bonart H, Schür MT, Hardt S, et al. Spontaneous charging affects the motion of sliding drops. *Nature Physics*. 2022;18(6):713-9.
2. Wong WSY, Bista P, Li X, Veith L, Sharifi-Aghili A, Weber SAL, Butt H-J. Tuning the Charge of Sliding Water Drops. *Langmuir*. 2022;38(19):6224-30.
3. Li X, Bodziony F, Yin M, Marschall H, Berger R, Butt H-J. Kinetic drop friction. *Nature communications*. 2023;14(1):4571.
4. Shumaly S, Darvish F, Li X, Saal A, Hinduja C, Steffen W, et al. Deep Learning to Analyze Sliding Drops. *Langmuir*. 2023.
5. Shumaly S. 4S-SROF toolkit <https://github.com/AK-Berger/4S-SROF2023> [

**Hauptautoren:** SHUMALY, Sajjad (Max Planck institute for polymer research); DARVISH, Fahimeh (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); LI, Xiaomei (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); KUKHARENKO, Oleksandra (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); STEF-

FEN, Werner (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); BUTT, Hans-Juergen (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany); BERGER, Ruediger (Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany)

**Vortragende(r):** SHUMALY, Sajjad (Max Planck institute for polymer research)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 4

Typ: **Poster**

## Elastohydrodynamic Coupling at the micro/nano scale

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

Soft and wet contacts are ubiquitous across scales from geology to physiology and are crucial for engineering. Interestingly, when an object moves near a soft substrate, the generated hydrodynamic pressure would deform the substrate, then resulting in the hydrodynamic coupling. Based on the EHD coupling, we proposed a contactless way to probe the mechanical properties of soft substrate using the colloidal atomic force microscopy. For instance, we use this contactless method to studies the viscoelasticity of the soft PDMD gels. Furthermore, when there is a parallel relative motion between the object and the soft substrate, a lift force will be generated normal to the direction of the motion because of the EHD coupling. Here we also present the first direct measurement of the EHD lift force using the AFM.

**Hauptautor:** ZHANG, zaicheng (University of Konstanz)

**Vortragende(r):** ZHANG, zaicheng (University of Konstanz)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 5

Typ: **Poster**

## Electrical Discharge of Sliding Drops

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

Water drops moving on many surfaces experience electrical charge separation. This process leads to opposite charging of the surfaces and drops, which changes properties of this system. Electrostatic forces affect the dynamic contact angles and sliding velocity of drops.[1] In addition, charges on the surface decreases its surface energy. Recently, charging of water drops inspires many researchers to design power generation devices and drop manipulation strategies.[2,3] Current research focuses mainly on the generation and accumulation process of charges. However, how do charged drops discharge?

We designed substrates with heterogeneous permittivity properties and coated them with an electrical insulating hydrophobic polymer. When a charged drop approaches the high permittivity substrate area, the electric field strength at the contact line exceeds the dielectric strength of the polymer coating. The latter leads to partial discharge of the drop. The discharge of the drop is associated with the formation of a Taylor cone at advancing contact line, resulting in a sharp decrease of advancing contact angle. Then, as the discharge process ends, the charges in the drop returns to zero. At the same time the Taylor cone, the local electric and the electrostatic force acting on the drop disappear. The dynamic contact angles are no longer affected by Maxwell stress and increase again. After the drop discharged, the charge separation at the receding contact line is enhanced. Thus, locally more charges are present, which increases the surface energy effectively.

The above charge-discharge-charge behaviour of the initial drop at the high permittivity substrate area affects the charging and sliding behaviour of subsequent drops. Controlling the charging and the discharging behaviour locally, allows us to manipulate drops. Understanding the discharging behaviour of sliding drops is the basis to improve slide electrification processes.

[1] Li, X. et al. Spontaneous charging affects the motion of sliding drops. *Nature Physics* 18, 713-719 (2022).

[2] Sun, Q. et al. Surface charge printing for programmed droplet transport. *Nature Materials* 18, 936-941 (2019).

[3] Xu, W. et al. A droplet-based electricity generator with high instantaneous power density. *Nature* 578, 392-396 (2020).

**Hauptautor:** NI, Zhongyuan (Max Planck Institute for Polymer Research)

**Co-Autoren:** LI, Xiaomei; BERGER, Rüdiger; Prof. BUTT, Hans-Jürgen

**Vortragende(r):** NI, Zhongyuan (Max Planck Institute for Polymer Research)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 6

Typ: **Poster**

## Electro(de)wetting with Photoswitches: Control of wetting by electric fields and light

Montag, 4. Dezember 2023 18:10 (20 Minuten)

Electro-dewetting (EDeW) was introduced as a new method in order to change the wetting properties of surfaces. Using ionic surfactants such as dodecyl tetraethyl ammonium bromide (DTAB) the wettability of hydrophilic silicon oxides on a conductive Si substrate can be controlled by an applied electrode potential, which leads to an increase in the contact angle. This behavior critically depends on the pH of the aqueous solution, the surfactant concentration and the potential used to drive EDeW. [1] The underlying mechanism is, however, not fully understood and additional experiments are needed.

In this contribution, we report on EDeW experiments using classical DTAB surfactants which confirm previous results [1], while we also report on the application of new cationic photoswitchable surfactants namely azobenzene triethylammonium bromide (Azo-TB) [2], arylazopyrazole triethylammonium bromide (AAP-TB) [2] and butyl-arylazopyrazole triethylammonium bromide (butyl-AAP-TB) for EDeW. These photoswitches can undergo E/Z photoisomerization reactions that cause drastically changes in surface activity [2,3] and offer the possibility to change the contact angle through light irradiation and to fine tune the EDeW ability of these systems. In previous work, [1] it was suggested that surfactants are deposited on the silicon oxide surface through the EDeW process. In order to study the suggested deposition of surfactants and the role of a possible prewetting layer outside of the contact line as a function of applied potential we have performed vibrational sum-frequency generation (SFG), which we combine with contact angle goniometry and ellipsometry, which are done in separate experiments. Ellipsometry is applied to monitor the thickness changes outside the drop at some distance from the 3-phase contact line and related to the results from vibrational SFG spectroscopy.

**Acknowledgements:** The authors gratefully acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) ∅ Project ID 3160439400 within the priority program SPP 2171 "Dynamic Wetting of Flexible, Adaptive and Switchable Substrates". The authors are also grateful for helpful discussions and support by MSc. Bas ter Beest (U Twente) and Prof. Dr. Frieder Mugele (U Twente).

[1] J. Li, Noel. S. Ha, T 'Leo' Liu, R. Michael van Dam, 'CJ' Kim. Nature 2019, 572, 507–510.

[2] M. Schnurbus, R. A. Campbell, J. Droste, C. Honnigfort, D. Glikman, P. Gutfreund, M. R. Hansen, B. Braunschweig, J. Phys. Chem. B., 2020, 124, 6913–6923.

[3] M. Hardt, F. Busse, S. Raschke, C. Honnigfort, J. Carrascosa-Tejedor, P. Wenk, P. Gutfreund, R. A. Campbell, A. Heuer, B. Braunschweig. Langmuir, 2023, 39, 5861-5871.

**Hauptautoren:** Frau SHAKHAYEVA, Billura (Universität Münster); BRAUNSCHWEIG, Björn

**Vortragende(r):** Frau SHAKHAYEVA, Billura (Universität Münster)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 7

Typ: **Talk**

## Thickness of nano-scale poly(dimethylsiloxane) layers determines the motion of sliding water drops

*Mittwoch, 6. Dezember 2023 12:20 (25 Minuten)*

Nanometer thick layers of polydimethylsiloxane (PDMS) are widely applied as hydrophobic coatings because they are environmentally friendly and chemically inert. In many applications, low friction of water drops is required. While the onset of motion (static friction) has already been studied, dynamic friction is less explored. It is not understood which processes lead to energy dissipation and cause friction. Such knowledge is important to minimize drop friction for applications such as heat exchangers or fog harvesting. Here, we measure dynamic friction of water drops on PDMS layers with different thickness and architecture over the whole available velocity regime. The layer thickness  $L$  turned out to be a good predictor for drop friction. 4-5 nm thick PDMS layers showed the lowest dynamic friction. A certain minimal layer thickness seems to be necessary to form homogeneous surfaces and reduce the attractive interaction between water and the underlying substrate. The increase of friction above  $L = 4-5$  nm is attributed to meniscus formation at the contact line due to the surface tension of water. When the contact line moves, the meniscus is dragged across the surface. Energy is dissipated due to stretching of chains and viscous dissipation. AFM force and friction experiments support this interpretation. The effect may be enhanced due to an increasing viscosity of the PDMS layer caused by entanglement of the polymer chains.

**Hauptautoren:** BUTT, Hans-Jürgen (Max Planck Institute for Polymer Research); KOYNOV, Kaloian; AMANN-WINKEL, Katrin; SUDERSAN, Pranav; BERGER, Rüdiger; LI, Xiaomei; ZHOU, Xiaoteng (Max Planck Institute for Polymer Research); WANG, Yongkang; NAGATA, Yuki

**Vortragende(r):** ZHOU, Xiaoteng (Max Planck Institute for Polymer Research)

**Sitzung Einordnung:** Short Talks



Beitrag ID: 8

Typ: Talk

## Dynamic Wetting and Electro-Dewetting with Photoswitchable Arylazopyrazoles

Dienstag, 5. Dezember 2023 17:00 (25 Minuten)

In this contribution, we provide information on photo-switchable self-assembled monolayers (SAMs) with fluorinated arylazopyrazole ( $\text{CF}_3$ -AAP) silanes on silicon oxide [1]. We have studied the molecular kinetics of the photoswitching in the SAMs in detail using both vibrational SFG and dynamic contact angle measurements. For that, we have systematically changed the surface coverage of the AAP photoswitches. The molecular kinetics of the wetted and pristine monolayer are surprisingly slow and the wetting dynamics are even slower when the SAM is closely-packed, which we relate to a coupling between the molecular kinetics and the drop dynamics. As we will show, the packing density of the SAMs and the possibility to incorporate water molecules into the SAM can have drastic influence on the wetting dynamics of  $\text{CF}_3$ -AAP monolayers. In addition, we have now extended our investigations to electro-dewetting (EDeW) experiments where we replace classical DTAB surfactants used in the original experiments (see Ref. [2]) by arylazopyrazole triethylammonium bromide (AAP-TB) which is a cationic amphiphile that can change the surface tension at the air-water interface to a large extent [3]. This offers to finetune the contact angle changes by E/Z photoisomerization of the AAP-TB amphiphile and we find a further increase in contact angle by about  $6^\circ$  when the samples were irradiated by UV light that triggers the photoisomerization from the E to the less surface active Z isomer. In previous work [2], it was suggested that surfactants are deposited on the silicon oxide surface through the EDeW process. In order to study the possible deposition of surfactants and the role of a possible prewetting layer outside of the drop and at some distance from the 3-phase contact line we have done SFG spectroscopy and find that surfactants are deposited even several mm adjacent to the drop and that the structure of this surfactant layer as well as the structure of the accompanying water layer changes drastically close to the 3-phase contact line.

**Acknowledgements:** The authors gratefully acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), Projects 422792175 and 422879009, within the priority program SPP2171 “Dynamic Wetting of Flexible, Adaptive and Switchable Substrates.”

[1] M. Golomb, N. B. Arndt, C. Honnigfort, B. Shakhayeva, B. J. Ravoo, B. Braunschweig; J. Phys. Chem. C 127, pp. 15316–15325 (2023).

[2] J. Li, Noel. S.Ha, T 'Leo' Liu, R. Michael van Dam, 'CJ' Kim; Nature 572, 507–510 (2019).

[3] M. Schnurbus, R. A. Campbell, J. Droste, C. Honnigfort, D. Glikman, P. Gutfreund, M. R. Hansen, B. Braunschweig; J. Phys. Chem. B. 124, 6913–6923 (2020).

**Hauptautoren:** SHAKHAYEVA, Billura; BRAUNSCHWEIG, Björn

**Vortragende(r):** BRAUNSCHWEIG, Björn

**Sitzung Einordnung:** Short Talks

Beitrag ID: 9

Typ: **Talk**

## Numerical simulation of droplets on membranes

*Montag, 4. Dezember 2023 14:45 (30 Minuten)*

Biological cells use membranes and droplets to compartmentalize their interior. As every structure within a cell is either enclosed by a membrane or by a liquid interface it is fundamental to ask what happens if these two come into contact. Recent studies suggest that membrane-droplet interactions are involved in various key biological processes. As experimental image resolution is limited at the corresponding length and time scales, we provide a first numerical method to shed some light on the dynamics on the process.

We derive a mathematical model to describe the interplay of an thin elastic membrane with a two-phase fluid. Using a combination of sharp and diffuse interface models, we develop a robust numerical strategy for this 3-phase multiphysics problem. The model is validated by analytical solutions of stationary morphologies. Finally, we demonstrate that the interplay between wetting dynamics and membrane elasticity leads to a range of fascinating phenomena like droplet wrapping, endocytosis and an inverted cheerios effect.

**Hauptautoren:** ALAND, Sebastian; MOKBEL, Marcel

**Vortragende(r):** ALAND, Sebastian

**Sitzung Einordnung:** Short Talks

Beitrag ID: 10

Typ: **Talk**

## Wetting of cytosolic protein condensates

*Mittwoch, 6. Dezember 2023 16:45 (20 Minuten)*

Protein condensates inside human cells are liquid-like droplets composed of protein and RNA. These condensates interact with the heterogeneous, active and dense environment of the cytoplasm, crossed by various cytoskeletal filaments such as microtubules and actin. Wetting interactions with the cytoskeleton lead to stereotypical positioning of such protein droplets inside the cell. Using statistical physics approaches, we identified complementary functions of filamentous actin and microtubules: protein droplets couple to actin's native dynamics in the cell through steric interactions leading to directional motion towards the cell center. Microtubules (and their molecular building-blocks), on the other hand, act as Pickering agents and engage in energetically favorable wetting interactions that lead to a robust localization of protein condensates in microtubule-rich regions of the cell. These interactions are non-specific and ultimately arise from different affinities (contact angles) between condensate and filament, suggesting that similar mechanisms may govern localization of other liquid-like phases within the cell.

**Hauptautor:** BÖDDEKER, Thomas (ETH Zurich / HU Berlin)

**Co-Autor:** DUFRESNE, Eric (ETH Zurich / Cornell University)

**Vortragende(r):** BÖDDEKER, Thomas (ETH Zurich / HU Berlin)

**Sitzung Einordnung:** Short Talks

Beitrag ID: 11

Typ: **Poster**

## Photoresponsive Polymer Brushes

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

Four polymer brush coatings containing photoresponsive arylazopyrazole (AAP)-based methacrylate monomers are reported. The glass substrates were functionalized using microcontact printing ( $\mu\text{CP}$ ) and surface-initiated atom transfer radical polymerisation (SI-ATRP). These polymer thin films were characterised by atomic force microscopy (AFM) and resulted in a height of 15 to 25 nm depending on the monomer composition. UV/*vis* and NMR spectroscopy confirmed the incorporation of the AAP-based monomers in the polymer brushes. Utilizing the photoisomerisation of the AAP, various characteristics of the surfaces can be tuned, specifically the wetting behaviour of the substrates can be reversibly switched, which was investigated via contact angle measurements.

**Hauptautor:** LOHRMANN, Steffen (University Münster)

**Co-Autor:** RAVOO, Bart Jan

**Vortragende(r):** LOHRMANN, Steffen (University Münster)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 12

Typ: **Talk**

## Charge deposition by moving contact lines reduces contact angles

*Montag, 4. Dezember 2023 15:15 (30 Minuten)*

Slide electrification-spontaneous charge separation at receding contact line has been reported to result in an electrostatic potential of around 1 kV and significantly affect drop motion. In order to find out how slide electrification influences contact angle, we examined the dynamic contact angles of aqueous droplets at various salt concentrations sliding down surfaces. We compare drops sliding down insulated surfaces for cases where the drop can charge up and cases where the drop is grounded along the entire drop pathway. This comparison exhibits that two electrification effects play a role in the reduction of dynamic contact angles: (a) the well-known reduction in contact angles, owing to electrowetting effects. (b) A decrease in receding contact angle owing to free surface energy changes of the solid at the rear side as a result of surface charge deposition. The latter effect changes surface energy in the order of 10 mN/m, leading to a substantial change in contact angle ( $\sim 10^\circ$ ), which should be considered in many works dealing with contact angle hysteresis on dielectric substrates.

**Hauptautoren:** LI, Xiaomei (Max-Planck-Institut für Polymerforschung); BUTT, Hans-Jürgen; Herr RATSCHOW, Aaron (TU Darmstadt); Prof. HARDT, Steffen (TU Darmstadt)

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

**Sitzung Einordnung:** Short Talks

Beitrag ID: 13

Typ: **Poster**

## Measuring Adaptation of pH-Sensitive Poly[2 (Dimethylamino)ethyl Methacrylate] Films

*Montag, 4. Dezember 2023 16:50 (20 Minuten)*

Adaptation may play a role in materials science, biology, and engineering<sup>1, 2</sup>. Dynamic adaptation is more relevant than static wettability due to allowing for greater versatility, functionality, and control over surface properties<sup>3</sup>. The dynamic adaptation process of liquids on solid surfaces is a complex subject due to its involvement with different lengths and time scales<sup>4, 5</sup>. The challenge becomes even bigger for adaptive or responsive surfaces<sup>6, 7</sup>. This is because responsive surfaces are often very sensitive to environmental changes. Ensuring consistent performance under different conditions is very difficult.

However, there is currently limited research exploring the dynamic adaptation and kinetics of moving droplets on pH-responsive surfaces<sup>8</sup>. When a surface displays hydrophilic characteristics coupled with significant contact angle hysteresis, the resistive force overcomes gravitational force. Therefore, gravitational forces alone prove inadequate in initiating droplet movement. Static measurements are susceptible to sensitivity issues, as placing a drop on the surface results in a contact angle between the advancing and receding values. Consequently, effective surface adaptation must be both robust and rapid to minimize the contact angle. As a result, the currently available methods for assessing surface adaptation remain limited.

Our method employing a Titled-plate setup involved a pump to deposit droplets of varying pH onto inclined polymer surfaces and a high-speed camera to record. It allows us to facilitate and analyze contact line movement. We selected a pH-responsive polymer made from (2-(Dimethylamino)ethyl methacrylate (PDMAEMA) as a representative surface. PDMAEMA is pH sensitive with a surface charge zero point occurring at a pH of 7.6. We employed the Atom Transfer Radical Polymerization (ATRP) method to prepare polymer brushes on both flat silicon substrates and rough glass substrates. In this study, we pioneered the investigation of dynamic adaptability in liquid droplets with varying pH levels on both horizontal and inclined polymer surfaces using two distinct methods.

### References

- (1) Butt, H.-J. r.; Berger, R. d.; Steffen, W.; Vollmer, D.; Weber, S. A. Adaptive wetting—adaptation in wetting. *Langmuir* 2018, 34 (38), 11292-11304.
- (2) Wong, W. S.; Hauer, L.; Naga, A.; Kaltbeitzel, A.; Baumli, P.; Berger, R. d.; D'Acunzi, M.; Vollmer, D.; Butt, H.-J. r. Adaptive wetting of polydimethylsiloxane. *Langmuir* 2020, 36 (26), 7236-7245.
- (3) Öner, D.; McCarthy, T. J. Ultrahydrophobic surfaces. Effects of topography length scales on wettability. *Langmuir* 2000, 16 (20), 7777-7782.
- (4) Bormashenko, E. Y. *Wetting of real surfaces*; Walter de Gruyter GmbH & Co KG, 2018.
- (5) Ras, R. H.; Marmur, A. *Non-wettable surfaces: theory, preparation and applications*; Royal Society of Chemistry, 2016.
- (6) Luzinov, I.; Minko, S.; Tsukruk, V. V. Adaptive and responsive surfaces through controlled reorganization of interfacial polymer layers. *Progress in Polymer Science* 2004, 29 (7), 635-698.
- (7) Bryuzgin, E.; Hyakutake, T.; Navrotsky, A.; Nishide, H.; Novakov, I. Control of surface wetting via production of graft polymer chains with adaptive behavior. *Protection of Metals and Physical Chemistry of Surfaces* 2013, 49, 101-108.
- (8) Li, X.; Auepattana-Aumrung, K.; Butt, H.-J.; Crespy, D.; Berger, R. Fast-release kinetics of a pH-responsive polymer detected by dynamic contact angles. *The Journal of Chemical Physics* 2023, 158 (14).

**Hauptautor:** JI, Yuwen (Max-Planck-Institut für Polymerforschung)

**Co-Autoren:** LEIBAUER, Benjamin (Max-Planck-Institut für Polymerforschung); SHUMALY, Sajjad (Max-Planck-Institut für Polymerforschung); BUTT, Hans-Jürgen (Max-Planck-Institut für Polymerforschung); BERGER, Rüdiger (Max-Planck-Institut für Polymerforschung)

**Vortragende:** JI, Yuwen (Max-Planck-Institut für Polymerforschung); BERGER, Rüdiger (Max-Planck-Institut für Polymerforschung)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 14

Typ: **Talk**

## **RHEOLOGY OF POLYMER SOLUTION DETERMINES THE EARLY STAGE OF THE DROP SPREADING**

*Dienstag, 5. Dezember 2023 11:30 (25 Minuten)*

Spreading of drops over solid substrate plays an important role in many industrial and natural systems. These systems are important for applications from printing and coating to agriculture. For low viscosity liquids, e.g. water, it is known that spreading consists of two regimes; inertia dominated regime and viscous dominated one. During the inertia regime, the spreading radius increases with the square root of time ( $r \sim t^{1/2}$ ). Thereafter, the spreading rate decreases into the viscous regime ( $r \sim t^{1/10}$ ).

Additionally, for liquids that are more viscous e.g. mixture of water and glycerin, the first steps of spreading slightly deviates from the square root of time law and the time exponent depends more on the wettability of the surface. The early stage of spreading happens in few milliseconds, which leads to high spreading velocity and a region high shear close to the contact line. We correlate the shear rate-dependent rheological properties of the drop to the dynamics of drop spreading. We use solution of water and PEO (Polyethylene Oxide) as shear thinning liquids and mixture of water and glycerin as the Newtonian liquid. At the same zero shear viscosity, viscoelastic (shear-thinning) drops spreads faster than a Newtonian drop. We discuss the influence molar mass and concentration of the polymer on the dynamics of drop spreading and give a qualitative model to describe the influence of shear-rate dependent viscosity on drop spreading.

**Hauptautor:** ROSTAMI, Peyman

**Co-Autoren:** SCHUBOTZ, Simon; Herr AZIZMALAYERI, Reza (Leibniz-Institut für Polymerforschung Dresden e.V.); Dr. AUERNHAMMER, Günter K.

**Vortragende(r):** ROSTAMI, Peyman

**Sitzung Einordnung:** Short Talks



Beitrag ID: 15

Typ: **Poster**

## Studying the surface charge density as the contact line dewets the surface

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

Charge separation in liquid drops sliding over a hydrophobized insulator surface is a well-known phenomenon and lots of efforts have been made to harness this effect for energy harvesting. However, a comprehensive understanding of the local surface charge density,  $\sigma$ , left behind by the sliding drop (receding contact line) is still lacking. Moreover, the behavior of surface charge density as multiple drops slide down the substrate is not fully understood. To close this gap of knowledge, we use a method based on mirror charge detection to locally measure surface charge density as drops dewet the hydrophobic surface. For this purpose, we positioned a metal electrode beneath the hydrophobic substrate to measure the capacitive current and by analyzing this current, we investigated the surface charge density left on different dielectric surfaces and studied the surface neutralization processes. Our observations indicate that around 20-30% of solid-liquid surface charge density from the electric double layer (EDL) is left on the surface. The surface neutralizes over time and the neutralization time,  $\tau$ , is influenced by the substrate and the surrounding environment. We present an analytical model that connects the solid-liquid surface charge to solid-air surface charge, which offers insights into the surface charge neutralization and gives the relevant parameters. Understanding these parameters and refining them could aid in optimizing the efficiency of solid-liquid charge separation.

**Hauptautor:** BISTA, Pravash

**Co-Autoren:** WEBER, Stefan; BUTT, Hans-Jürgen

**Vortragende(r):** BISTA, Pravash

**Sitzung Einordnung:** Poster Session

Beitrag ID: 16

Typ: **Talk**

## Droplet on soft flexible sheets

*Dienstag, 5. Dezember 2023 12:20 (25 Minuten)*

Leveraging our established droplet model developed using the boundary element method (BEM), we investigate dynamic wetting on thin flexible sheets. One promising application arising from this research is the potential for designing tunable fluidic lenses.

Central to our study is the nuanced interplay between the mechanical attributes of the sheet and droplet behavior, with a particular emphasis on contact angle during wetting. Drawing inspiration from biological membranes, we have integrated the Skalak model for elastic deformations and the Helfrich Hamiltonian for bending mechanics into our approach. This enables us to dissect how tension forces and sheet rigidity impact droplet shape and wetting dynamics. While our findings have implications for material science, they are equally significant for biological applications, illuminating the fascinating interactions between soft substrates and liquid interfaces.

**Hauptautoren:** SULTAN, Salik (TU Berlin); Prof. STARK, Holger (TU Berlin)

**Vortragende(r):** SULTAN, Salik (TU Berlin)

**Sitzung Einordnung:** Short Talks

Beitrag ID: 17

Typ: **Poster**

## Control of the water flux by variation of the interlamellar distance

Montag, 4. Dezember 2023 18:10 (20 Minuten)

The manipulation with topography of surfaces, which can be achieved through the application of external stimuli, including temperature, magnetic fields, pH, light, and others stimuli, allows switching of wetting and adhesion. Shape-memory polymers is one kind of materials can alter their appearance under applied stress and can be used for fabrication of such smart surfaces. Particularly, thermo-responsive shape memory polymers can revert to their original structure after a thermal cycle involving heating, cooling, and reheating. Additionally, two-way actuation polymers can change their shape by adjusting the temperature in a stress-free regime. An intriguing example of such materials is poly(1,4-butylene adipate)-based poly(ester urethane) (PEU-PBA). During a thermal-mechanical pretreatment, the PEU-PBA contains regions which may crystallize at temperatures below 8°C, leading to a change in the polymer's shape [1]. Thermal-responsive polymers provide precise control over their shape through temperature manipulation, making them valuable for regulating fluid flow processes.

In our study, we employed polyurethane with poly(1,10-decylene adipate) as the soft segment [2]. We fabricated a lamellar structure with a height of approximately 1.5 mm and an interlamellar distance of 2 mm by using the melt-electrowriting technique at a temperature of 200°C and an applied voltage of 3kV. These lamellae can change their shape when heated due to expansion and decrystallization effects, and this transformation is reversible. By adjusting the temperature, we can effectively control the volume between neighboring lamellae. The presence of a water droplet between two lamellae reduces the volume between them until they collapse. After evaporation, the space between the two lamellae is maintained. Furthermore, we can restore or modify the volume of the collapsed channel by adding another droplet between the collapsed lamella and the non-collapsed one. Varying the temperature enhances the flexibility of our lamellae, allowing us to modulate the fluid flow by altering the temperature and adjusting the surface tension of water. This characteristic opens up exciting possibilities for utilizing such topographies in microfluidic devices and for creating new materials for tubing fabrication.

[1] Martin Bothe and Thorsten Pretsch Bidirectional actuation of a thermoplastic polyurethane elastomer// J. Mater. Chem. A, 2013, 1, 14491–14497.

[2] Schönfeld, D.; Chalissery, D.; Wenz, F.; Specht, M.; Eberl, C.; Pretsch, T. Actuating Shape Memory Polymer for Thermo-responsive Soft Robotic Gripper and Programmable Materials// Molecules 2021, 26, 522.

**Hauptautor:** SADILOV, Ilia (University of Bayreuth, Bayreuth, Germany)

**Co-Autoren:** CONSTANTE, Gissela (University of Bayreuth, Bayreuth, Germany); SCHÖNFELD, Dennis (Fraunhofer Institute for Applied Polymer Research IAP, Potsdam, Germany); PRETSCH, Thorsten (Fraunhofer Institute for Applied Polymer Research IAP, Potsdam, Germany); IONOV, Leonid (University of Bayreuth, Bayreuth, Germany)

**Vortragende(r):** SADILOV, Ilia (University of Bayreuth, Bayreuth, Germany)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 18

Typ: **Poster**

## Steering droplets on substrates with travelling wave wettability patterns and deformations

*Montag, 4. Dezember 2023 17:10 (20 Minuten)*

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 imposing a wettability pattern on the substrate [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 travelling wave wettability pattern by varying the speed and wave length of the pattern. Second, we investigate a droplet on substrates with a travelling wave height profile. In both scenarios, for small wave velocities the droplet moves steadily forward. In contrast, above a wave velocity the droplet performs steady oscillations. These speed oscillations correlate with oscillations in the shape of the droplet which decay linearly as a function of pattern speed.

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

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

**Sitzung Einordnung:** Poster Session

Beitrag ID: 19

Typ: Talk

# Synthesis and characterization of solvatochromic dye-gradient polymer brushes

Dienstag, 5. Dezember 2023 11:55 (25 Minuten)

## Synthesis and characterization of solvatochromic dye-gradient polymer brushes

Jonah Decker<sup>1</sup>, Sören Steup<sup>2</sup>, Sergey I. Druzhinin<sup>1</sup>, Heiko Ihmels<sup>2</sup>, Holger Schönherr<sup>1\*</sup>

<sup>1</sup> Physical Chemistry I, Department of Chemistry and Biology and Research Center of Micro and Nanochemistry and (Bio)Technology (Cμ), University of Siegen

<sup>2</sup> Organic Chemistry II, Department of Chemistry and Biology and Research Center of Micro and Nanochemistry and (Bio)Technology (Cμ), University of Siegen

E-mail: schoenherr@chemie.uni-siegen.de

In the project, the dynamics of wetting of the poly(di(ethyleneglycol) methyl ether methacrylate) (PDEGMA) brushes is studied by analysing the fluorescence dynamics of a solvatochromic reporter dye. In these brushes the dyes are coupled to the polymer chain and probe the local polarity in their vicinity [1]. Hence they can be applied as reporters for the local state of the chain hydration in the brush interior. This allows one to image the wetting dynamics with confocal fluorescence microscopy both with high lateral as well as significantly enhanced axial resolution. To achieve this, poly(di(ethyleneglycol) methyl ether methacrylate) brushes with an overall uniform height were successfully synthesised, containing a solvatochromic dye covalently attached to the brushes in a one-dimensional depth gradient. Two consecutive steps of gradient brush synthesis via surface-initiated activator regenerated by electron transfer atom transfer radical polymerization (SI-ARGET ATRP) were performed with inverse gradient directions to realize this unique brush architecture [2]. Between those two steps, a short segment of a co-monomer, containing the solvatochromic dye covalently attached to di(ethyleneglycol) methyl ether methacrylate (DEGMA) was polymerized. In this contribution, the synthesis and characterization of > 200 nm thick polymer brush systems with a short dye-containing co-monomer segment with a one-dimensional gradient inside will be presented. Fluorescence lifetime imaging microscopy measurements of polymer brushes in dry and wet conditions will also be discussed.

The authors gratefully acknowledge the financial support by the Deutsche Forschungsgemeinschaft (DFG in the SPP 2171, SCHO 1124/8-1) and the University of Siegen.

### References

[1] A. Yadigarli, Q. Song, S. I. Druzhinin, H. Schönherr, Beilstein J. Org. Chem. 2019, 15, 2552.

[2] S. Großhans, I. Lilge, H. Schönherr, Macromol. Biosci. 2018, 18 (2), 1700317.

**Hauptautor:** DECKER, Jonah

**Co-Autoren:** Herr STEUP, Sören; Dr. DRUZHININ, Sergey I.; Prof. IHMELS, Heiko; Prof. SCHÖNHERR, Holger

**Vortragende(r):** DECKER, Jonah

**Sitzung Einordnung:** Short Talks

Beitrag ID: 20

Typ: **Poster**

## Slide electrification of water droplets over CYTOP electrets surfaces

Montag, 4. Dezember 2023 17:30 (20 Minuten)

Slide electrification of water droplets over CYTOP electrets surfaces

Shalini<sup>1,4</sup>, Dhiman Mallick<sup>1, 2</sup>, Rüdiger Berger<sup>4</sup> and Ankur Goswami<sup>1,3</sup>

<sup>1</sup>School of Interdisciplinary Research, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India <sup>2</sup>Department of

Electrical Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India

<sup>3</sup>Department of Material Science Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India

<sup>4</sup>Max Plank Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Keywords: Fluoropolymer, Charge trapping, Charge storage, Energy harvesting, KPFM/EFM.

Abstract

Drops sliding on surfaces can result in charging of drops and surfaces. Thus subsequent sliding drops can interact with charged surface differently[1]. Drops slide electrification effects are one way how surfaces adapt[2]. Fluorinated surfaces typically exhibit drop slide electrification phenomena. CYTOP is an amorphous hydrophobic fluoropolymer that can be used to create electret films. CYTOP finds plethora of applications in microelectronic devices for sustainable energy and memory devices which demands high voltage breakdown, high dielectric constant, and amorphous structure, transparency, and charge storage capabilities. Here, we present direct quantification and mapping of surface charge on CYTOP film at room temperature using advanced scanning probe microscopy (SPM) technique such as Kelvin Probe Force Microscopy (KPFM) and Electrostatic Force Microscopy (EFM)[3]. We calculated the surface charge densities are of  $0.7 \text{ } \mu\text{C}/\text{cm}^2$  and  $1.5 \text{ } \mu\text{C}/\text{cm}^2$  for positive and negative charges respectively which are injected at the certain areas on the surface employing the SPM tip by applying controlled bias voltages further, we have estimated the charge retention time for both positive and negative charges which are impinged on this polymer. We found that the retention capacity of the CYTOP film for the injected negative charges is much higher than the injected positive charges. In a next step we will investigate how injected charges influence the sliding behavior of drops.

References

[1] K. Yatsuzuka, Y. Mizuno, and K. Asano, "Electrification phenomena of pure water droplets dripping and sliding on a polymer surface," *Journal of Electrostatics*, vol. 32, no. 2, pp. 157-171, 1994/04/01 1994.

[2] X. Li et al., "Spontaneous charging affects the motion of sliding drops," *Nature Physics*, vol. 18, no. 6, pp. 713-719, 2022/06/01 2022.

[3] W. Melitz, J. Shen, A. C. Kummel, and S. Lee, "Kelvin probe force microscopy and its application," *Surface Science Reports*, vol. 66, 2011/01/01 2011.

- **List item**

**Hauptautoren:** SHALINI, shalini (PhD Student); Herr MALLICK, Dhiman (Professor); Herr BERGER, Rüdiger; Herr GOSWAMI, Ankur

**Vortragende(r):** SHALINI, shalini (PhD Student)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 21

Typ: **Talk**

## High Voltages Generated by Moving Water Drops

*Dienstag, 5. Dezember 2023 15:15 (25 Minuten)*

Water drops sliding on insulating, hydrophobic substrates can become electrically charged [1–3]. Despite many decades of research, this spontaneous electrification of moving drops is still far from being understood. By precisely measuring charge and voltage, we found that moving water drops accumulate a voltage of several kilovolts after sliding for just a few centimeters. To enable an efficient utilization of this simple electric energy generation mechanism, a detailed and quantitative understanding of the underlying physical process would be required. Using a simple electrostatic model, we show that the drop voltage is fundamentally connected to the properties of the electrostatic double layer at solid-liquid interfaces. The observation of high drop voltages will have important implications for energy harvesting applications, as well as droplet microfluidics and electrostatic discharge protection.

[1] A. Z. Stetten, D. S. Golovko, S. A. L. Weber, and H.-J. Butt, Slide Electrification: Charging of Surfaces by Moving Water Drops, *Soft Matter* 15, 8667 (2019).

[2] D. Díaz, D. Garcia-Gonzalez, P. Bista, S. A. L. Weber, H.-J. Butt, A. Stetten, and M. Kappl, Charging of Drops Impacting onto Superhydrophobic Surfaces, *Soft Matter* 18, 1628 (2022).

[3] X. Li et al., Spontaneous Charging Affects the Motion of Sliding Drops, *Nat. Phys.* 1 (2022).

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

**Co-Autor:** BISTA, Pravash

**Vortragende:** WEBER, Stefan (MPI for Polymer Research Mainz); BISTA, Pravash

**Sitzung Einordnung:** Short Talks

Beitrag ID: 22

Typ: **Poster**

## Water Sensing in Polymers by Time-Resolved Fluorescence of Solvatochromic Dye

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

We are interested in the analysis of the (de)hydration dynamics of polymer-coated surfaces monitored with time-resolved fluorescence microscopy. In particular, the reversible changes of the wetting state in thermally-switchable polymer layers is imaged in a confocal microscope via changes of the fluorescence intensity, spectrum and/or decay time of the reporter dye due to changes of local polarity. This may enable the direct detection of water molecules in the vicinity of the polymer chains. In this stage the fluorescence spectra and lifetimes of a solvatochromic dye (Nile red (NR) derivative) were measured in solvents of different polarity and in binary organic solvent/water mixtures mimicking wetted polymer layers on the surface. The absorption and fluorescence spectra of NR are significantly shifted to the red, when the solvent polarity increases. In protic solvents there is an additional substantial longwavelength shift compared to dipolar solvents of the same polarity due to specific interactions of NR with the solvent. The fluorescence lifetime of NR increases in polar solvents and decreases in protic solvents. To estimate the effect of solvent composition on the photophysical properties of the solvatochromic dye, absorption and fluorescence spectra, as well as fluorescence kinetics of NR were investigated in two binary solvent mixtures. One was a mixture of two dipolar aprotic solvents of the same polarity and another one was a mixture of aprotic and protic solvents also the same polarity. The direct detection of water was carried out by using hydroxy- and methoxy-substituted  $\beta$ -carboline. In the ground state these derivatives form complexes with water. While with OMe-derivatives only a minor change of fluorescence has been found, the OH-derivatives, being a photoacid, reacts with water leading to a drastic reduction of its fluorescence intensity and lifetime in the presence of water. The mechanism of this fluorescence quenching, static and/or dynamic, is discussed. In addition, to analyze the detection of the wetting state of the thermally-switchable poly(di(ethylene glycol) methyl ether methacrylate) (PDEGMA) layer on glass surfaces, the fluorescence spectra and decay of NR were measured in PDEGMA at different temperatures. With the fluorescence spectra of NR it was shown that PDEGMA layer has a moderate polarity between that of ethyl acetate and acetone. The fluorescence of NR in PDEGMA decays double exponentially with a major long-lived (4.6 ns) and a minor short-lived (2.1 ns) component. The PDEGMA brushes are wetted below 32°C and are dewetted above this temperature. When the temperature varies from 20 to 50°C, strong deswelling of PDEGMA (swelling ratio from 3 at 25°C to 1.5 at 50°C) is accompanied with a substantial reduction (from 0.22 to 0.12) of the contribution of the short-lived decay component of NR.

### Acknowledgment

The authors acknowledge financial support by DFG (SCHO 1124/7-1, IH24/17-1 and SPP 2171, SCHO 1124/8-1) and the University of Siegen.

**Hauptautoren:** 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); Herr 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); Herr DECKER, Jonah (Physical Chemistry I, Department of Chemistry and Biology and Research Center of Micro and Nanochemistry and (Bio)Technology (C $\mu$ ), University of Siegen); Herr GROSS, Philipp (Or-



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

**Vortragende(r):** 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)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 23

Typ: **Talk**

## High-Order Methods for Fluid-Soft Substrate Interactions with Heat Transfer and Evaporation

*Dienstag, 5. Dezember 2023 09:45 (25 Minuten)*

We introduce an advanced extended discontinuous Galerkin method (XDG) tailored for the simulation of multiphase problems including three-phase contact lines. This approach adeptly handles three-phase contact lines, especially evident when examining the interaction between water droplets and flexible solids such as silicone-gel. Utilizing the Navier slip boundary conditions coupled with Young's equation, we probe the intricacies of these interactions. An intrinsic challenge arises from the singularities observed at interfaces and three-phase contact lines, such as abrupt changes in pressure or surface tensions. High-order methods typically require smooth functions to achieve optimal convergence, which poses a challenge in these situations.

Within the first phase of the priority programme, a Euler-Lagrange approach was realized. For the second phase, where also Heat Transfer and Evaporation should be considered, we are transitioning to a Euler-Euler model. The representation of all properties within the same Euler frame allows a fully coupled solution, which benefits the numerical stability of the method.

We are going to present a deep and comprehensive comparison between the Euler-Lagrange and Euler-Euler models. Our analysis will not only present numerical results but also address the methodological underpinnings that prompted our transition from one model to the other. Furthermore, we are going to show first results on evaporation, with special emphasis on the modelling at the contact line.

**Hauptautoren:** MIAO, Chen; KUMMER, Florian (TU Darmstadt - FG Strömungsdynamik)

**Vortragende(r):** MIAO, Chen

**Sitzung Einordnung:** Short Talks

Beitrag ID: 24

Typ: **Talk**

## Stick-slip Contact Line Dynamics in Forced Wetting of Polymer Brushes

*Donnerstag, 7. Dezember 2023 09:45 (25 Minuten)*

We study the wetting of adaptive substrates using a mesoscopic hydrodynamic model for a liquid droplet on a polymer brush, refining the model in [1]. First, we show that Young's law still holds for the macroscopic equilibrium contact angle and that on the mesoscale a Neumann-type law governs the shape of the wetting ridge (comparable to the case of elastic substrates [2]). Further, we numerically examine the wetting ridge dynamics for a moving meniscus, i.e., we consider an "inverse Landau-Levich geometry" where a brush-covered plate is introduced into a bath. We find stick-slip motion in good qualitative agreement with experimental observations [3,4] and discuss criteria for the onset of the corresponding instability.

[1] U. Thiele and S. Hartmann, Eur. Phys. J.-Spec. Top., 2020, 229, 1819-1832.

[2] B. Andreotti and J. H. Snoeijer, Annu. Rev. Fluid Mech., 2020, 52, 285-308.

[3] S. Schubotz et al., Adv. Colloid Interface Sci., 2021, 294, 102442.

[4] L. Wan, X. Meng, Y. Yang, J. Tian and Z. Xu, Sci. China Chem., 2010, 53, 183-189.

**Hauptautor:** GREVE, Daniel

**Co-Autoren:** Dr. HARTMANN, Simon; THIELE, Uwe

**Vortragende(r):** GREVE, Daniel

**Sitzung Einordnung:** Short Talks

Beitrag ID: 25

Typ: **Poster**

## Intracellular wetting between biomembranes and liquid-like condensates

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

Wetting has been recently identified as physiologically important in fundamental cellular processes: phase-separated condensates (e.g., proteins and RNA) form liquid droplets in cells and interact with membranes, e.g., during autophagy in eukaryotic cells or protein storage in plant vacuoles. Upon contact, the droplets can exert wetting forces on the membrane that deforms. This creates a competition of mechanical forces of the membrane elasticity and the droplet capillarity, giving rise to elastocapillary phenomena. In this talk, I will present a minimal model system comprising giant lamellar vesicles (GUVs) filled with a phase-separating polymer system (PEG/Dextran). We create liquid-liquid interfaces inside GUVs by osmotic quenches, yielding deformed vesicles with excess membrane area. The excess membrane accumulates at the liquid-liquid interface and assumes differing morphologies, ranging from micro-tubules to sheets, to stomatocytes. We find that morphology transition depends on the liquid-liquid surface tension. Our results will help to explain resembling in vivo observations during the morphogenesis of protein storage vacuoles in plants.

**Hauptautoren:** HAUER, Lukas (Humboldt Universität); SPORBECK, Katharina; KNORR, Roland L.

**Vortragende(r):** HAUER, Lukas (Humboldt Universität)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 28

Typ: Talk

## Memory effects of PNiPAAm brushes in different atmospheres

Mittwoch, 6. Dezember 2023 11:30 (25 Minuten)

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.

In further wetting experiments we measure water drops in an ethanol-saturated atmosphere on PNiPAAm brushes. 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.

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

[2] Schubotz, S., et al., Influence of the Atmosphere on the Wettability of Polymer Brushes. *Langmuir* 2023, 39, 14, 4872–4880

**Hauptautoren:** SCHUBOTZ, Simon (Technische Universität Dresden); AUERNHAMMER, Günter K.; UHLMANN, Petra (Leibnitz-Institut für Polymerforschung, Dresden); FERY, Andreas (Technische Universität Dresden); SOMMER, Jens-Uwe (Technische Universität Dresden)

**Vortragende(r):** AUERNHAMMER, Günter K.

**Sitzung Einordnung:** Short Talks

Beitrag ID: 29

Typ: **Poster**

## Dynamic wetting of concentrated granular suspensions

Montag, 4. Dezember 2023 18:10 (20 Minuten)

Concentrated granular suspensions are employed in a variety of applications including 3D printing, painting, etc. In a wetting process, the contact line dynamics and the internal structure of the suspension interact. Along the contact line, particles interact with each other and the substrate. This process can be characterized using individual particle analysis and average suspension descriptions. There is a markedly high shear rate at the droplet's contact line. This localized shear rate profoundly affects suspension's non-Newtonian rheological behaviour.

Recent researches have affirmed the applicability of the hydrodynamic solutions like Cox-Voinov relation to granular suspensions, highlighting the importance of particles approaching the contact line area to influence the effective wetting viscosity. Despite these efforts, the impact of particles on the overall flow field and microstructure of densely packed granular systems along the contact line remains unexplored.

In this study, we use fluorescently labelled tracer particles in a refractive index-matched Silica suspension to investigate the flow field close to the contact line. Two distinct dispersion media are employed to study the significance of inter-particle interactions within our experimental framework. We utilize a configuration consisting of a pinned droplet on a moving substrate and by employing astigmatism particle tracking velocimetry (APTV), we precisely track the 3D motion of tracer particles within the concentrated suspension. Particle trajectories give the flow profile of a droplet near the advancing contact line. Furthermore, side-view images enable for the characterization of the drop shape. The dynamic response of the suspension to shear stresses is characterized using amplitude-sweep rheology measurements.

The angle of repose measurements demonstrates frictional contact between submerged particles. Near the advancing contact line, we observe distinct behaviours based on the interaction between particles resulting from the choice of dispersion medium. When using 2,2'-thiodiethanol (TDE) as the dispersion medium it leads to weakly interacting particles, the flow field indicates a violation of the hydrodynamic solutions like Cox-Voinov relationship, with particle friction becoming a significant factor. Conversely, when strong particle interactions are present, using sodium thiocyanate (NaSCN) salt solution as the dispersion medium, the suspension exhibits a yield stress behaviour. In this scenario, particles migrate toward the high shear rate zone near the contact line, and the suspension behaves more like a liquid close to the moving substrate, with particles approaching the contact line and moving parallel to it. These observations are substantiated by rheology and angle of repose measurements. Near the receding contact line, the suspension adheres to its previous layer and moves on top of it. This results in a dynamic curvature of the receding contact line, which undergoes a transient dynamic before reaching stationary state.

**Keywords:** Dynamic wetting, Granular suspensions, Rheology

**Hauptautoren:** ROSTAMI, Peyman; AZIZMALAYERI, Reza; WITZMANN, Thomas; KLEIN, Christopher; PATEL, Himanshu P.; AUERNHAMMER, Günter K.

**Vortragende(r):** AZIZMALAYERI, Reza

**Sitzung Einordnung:** Poster Session

Beitrag ID: 30

Typ: **Keynote**

## Dynamics of a deformable droplet enclosing active particles

*Dienstag, 5. Dezember 2023 14:30 (20 Minuten)*

Biological cells are dynamic systems that undergo complex transformations (e.g., division, growth, and translocation) in the absence of external control. Neutrophils of the immune system are a prime example of such complex, cell-autonomous locomotion. These cells exhibit directed motion as they sense and move towards bacteria while navigating a forest of red blood cells. An artificial system that mimics this type of behavior would hold enormous potential for the next generation of autonomous micro-robotic systems.

Recently, locomotion of non-living cell-like objects has been realized experimentally in my Lab

I will discuss our progress in understanding the mechanisms of the motility and role of

**Hauptautor:** VLAHOVSKA, Petia (Northwestern University)

**Vortragende(r):** VLAHOVSKA, Petia (Northwestern University)

**Sitzung Einordnung:** Keynote

Beitrag ID: 31

Typ: **Talk**

## Phase Separation in Wetting Ridges of Sliding Drops on Soft and Swollen Surfaces

*Mittwoch, 6. Dezember 2023 11:55 (25 Minuten)*

Drops on soft substrates can induce capillary-mediated phase separation of free polymer chains (oligomers) in wetting ridges. The separation is particularly interesting for moving ridges as the material makeup in the ridge governs friction dissipation and, hence, the drop dynamics. In this talk, I present drop-sliding experiments on soft PDMS gels (3-5 kPa) swollen with oligomeric silicone oil (10 to 16 times the dry network volume). The separation of oligomers at the ridge tip is resolved directly in time and space with confocal microscopy, and the differing phases (oligomers and gel) are discerned with differing fluorescence tags. We find that the two phases (oligomers and gel) separated to different degrees, depending on the sliding speed and the amount of swollen oil. A diffusion-advection model that considers the chemical potential in the respective phases is developed and validated with experimental data. The model helps to explain I) the degree of phase separation, and II) the mobility of the silicone oil in the PDMS network.

**Hauptautoren:** HAUER, Lukas; CAI, Zhuoyun; SKABEEV, Artem; PHAM, Jonathan T.; VOLLMER, Doris

**Vortragende(r):** HAUER, Lukas

**Sitzung Einordnung:** Short Talks



Beitrag ID: 32

Typ: **Talk**

## Size-Dependent Wetting of Microscopic Low-vapor Pressure Droplets on Smooth Silane-Coated Substrate

*Mittwoch, 6. Dezember 2023 15:50 (25 Minuten)*

The static contact angle of a liquid droplet on a substrate is often used to describe its wetting properties, which are influenced by various factors such as the chemistry of the substrate, properties of the liquid, and environmental conditions. Our study shows that the wetting of a microscopic droplet can systematically depend on its size. This dependency can be described with consideration of surface roughness, surface forces, and liquid surface tension. A smooth silane coating was produced using solvent-based silanization coupled with various post-treatment methods. To prevent evaporation during AFM scanning, different low-vapor pressure liquids, including Polyethylene glycol 200, Ethylene Glycol, and glycerol, were selected as the liquid phase and all measurements were carried out in a nitrogen environment to avoid water uptake. The static microscopic Contact Angle compared with the macroscopic Contact Angle, measured via an optical method. The results showed that the static Contact Angle increases by increasing drop size up to a limit, which depends on droplet surface tension. In addition, the microscopic contact angle was smaller than the macroscopic counterpart, which indicates the dominance of roughness forces at the contact line.

**Hauptautor:** HORMOZI, Mohammadali (TU Darmstadt)

**Co-Autoren:** Prof. VON KLITZING, Regine (TU Darmstadt); Herr ROSTAMI, Peyman (Leibniz-Institut für Polymerforschung Dresden e. V.)

**Vortragende(r):** HORMOZI, Mohammadali (TU Darmstadt)

**Sitzung Einordnung:** Short Talks

Beitrag ID: 33

Typ: Talk

## Enhancement of photoswitchable wetting properties of SP-containing porous surfaces by roughness adjustment

Mittwoch, 6. Dezember 2023 15:15 (25 Minuten)

The fabrication of smart surfaces with photoswitchable wetting properties is of great interest for applications such as coatings with various wetting patterns[1], photo-controlled liquid imbibition[2] or condensation[3]. Spiropyran (SP) stands out among the photoswitches due to the significant dipole moment change from SP to merocyanine (MC), featuring a remarkable color change upon UV exposure. Roughness, as a key parameter for the wetting behavior of a surface, needs to be adjusted to enhance the static contact angle (SCA) switch as well. However, common fabrication methods to fabricate SP functionalized surfaces with a suitable roughness have some drawbacks such as complicity and surface sensitivity.

In this work, synthesized SP monomer was incorporated into the bulk material, ensuring that the fabricated photoswitchable substrates remained functional after abrasion. A micro-/nanoscale roughness was introduced to the material via the polymerization-induced phase separation (PIPS) method [4] to amplify the SCA switch. Polymers with different roughness were achieved by varying the crosslinker content, as it influences the PIPS and shrinkage. SCA was measured on all the samples before and after UV exposure. According to our results, not only the SP but also the pore size (i.e. roughness) is a crucial parameter for tuning the photoswitchable wetting properties. For samples with larger pores, low roll-off (RA) angles and high SCA, indicate the dominance of the Cassie-Baxter state. This results in less SP/MC contact and hence, insignificant SCA change. While samples with smaller pores could provide SCA changes up to 161° as the Wenzel State would be dominant, allowing for a higher interface of SP/MC and the droplet. Samples with the highest SCA change also exhibited greater coalescence of condensed water droplets at the micro- and macroscale after UV exposure with lower hydrophobicity.

### References

- [1] H.S. Lim, J.T. Han, D. Kwak, M. Jin, K. Cho, J. Am. Chem. Soc. 2006, 128, 14458.
- [2] A. Nayak, H. Liu, G. Belfort, Angew. Chem. 2006, 118, 4200.
- [3] S. Feng, Y. Hou, Y. Xue, L. Gao, L. Jiang, Y. Zheng, Soft Matter 2013, 9, 9294.
- [4] D. Helmer, N. Keller, F. Kotz, F. Stolz, C. Greiner, T.M. Nargang, K. Sachsenheimer, B.E. Rapp, Sci Rep 2017, 7, 15078.

**Hauptautoren:** NEKOONAM, Niloofar; DREHER, Franziska (University of Freiburg); HELMER, Dorothea (University of Freiburg)

**Vortragende(r):** NEKOONAM, Niloofar

**Sitzung Einordnung:** Short Talks

Beitrag ID: 34

Typ: **Talk**

## The breakup dynamics of viscous capillary bridges on hydrophobic surfaces

*Mittwoch, 6. Dezember 2023 09:45 (25 Minuten)*

The breakup dynamics of highly viscous capillary bridges on grounded hydrophobic surfaces is investigated. The breakup dynamics bears a very close resemblance to that of highly viscous free capillary bridges. However, due to the strong dependency of the dynamics on the surface properties, the wettability of the substrate must be taken into account. In this regard, it is demonstrated that under specific conditions, particularly for hydrophobic surfaces and slow dynamics, inertia and hydrodynamic dissipation in the bulk can be disregarded. In view of this, a simple scaling law based on the balance between surface forces and contact line friction force (according to the Molecular Kinetic Theory) is derived. Furthermore, Surface Evolver is employed to calculate the shape of the capillary bridge under various geometrical constraints before breakup. It is shown that the minimum width of the capillary bridge at the onset of instability is the correct length scale for the problem at hand. Accordingly, the correct time and velocity length scales are computed, leading to scaling variables that let groups of experimental data collapse on the same curve.

**Hauptautor:** JABBARY FARROKHI, salar (TU Darmstadt)

**Co-Autor:** Prof. HARDT, Steffen (nstitute for Nano- and Microfluidics, TU Darmstadt, Alarich-Weiss-Straße 10, D-64237 Darmstadt, Germany)

**Vortragende(r):** JABBARY FARROKHI, salar (TU Darmstadt)

**Sitzung Einordnung:** Short Talks

Beitrag ID: 35

Typ: **Poster**

## Responsive Water Pinning in Liquid Crystal Elastomers

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

Liquid crystal elastomers (LCEs) are an exceptional framework for highly active and functional soft matter. Briefly, LCEs couple the anisotropic LC director to a soft polymer network resulting in a zoo of phase-dependent responsive properties including reversible optical switching, mechanical stiffening, and shape-shifting in response to heat, light, or magnetic/electric fields. Here, we obtain reversible surface instabilities in LCEs with large amplitude features that are strikingly similar to that of rose petals and display temperature-responsive water pinning properties. Further, the ability to program arbitrary shape-changes, such as a smooth film that morphs into a replica of a lupin leaf, offers a route to cheaply and quickly produce functional surface roughening for wetting applications.

**Hauptautor:** BARNES, Morgan (University of Cambridge)

**Co-Autoren:** Dr. FENG, Fan (University of Cambridge); Prof. BIGGINS, John (University of Cambridge)

**Vortragende(r):** BARNES, Morgan (University of Cambridge)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 36

Typ: Talk

## Electrified droplets between horizontal cylinders

*Donnerstag, 7. Dezember 2023 11:25 (25 Minuten)*

A liquid bridge is a liquid droplet suspended between solid surfaces. We study pendant liquid bridges between two horizontally aligned cylindrical rods using experiments, direct numerical simulations and reduced-order model equations obtained by minimizing an appropriate Rayleighian according to Onsager's variational principle. Additionally, we analyse the influence on the dynamics of perfect dielectric liquid bridges of the electric field resulting from an imposed potential difference between cylindrical electrodes. Our findings reveal that the electric field pulls the liquid upwards and flattens the liquid-air interfaces. Also, we find that the maximum trapping capacity (i.e. the amount of fluid that can be captured between the cylinders) is increased in the presence of the electric field. The experiments are performed using silicone oil droplets and three types of cylindrical electrodes: titanium, copper, and stainless-steel rods. We observe that the experimental results are well described by the model equations for a wide range of parameter values.

Since liquid bridges are a reasonably good models of Plateau border cross-sections in a liquid foam, by understanding the dynamics in such geometry, we gain better insight in electrohydrodynamics phenomena in foams. Thus, this project is contributing to tackling key problems related to the control and stability of liquid foams.

**Hauptautor:** BOKANYI-TOTH, Agnes (Loughborough University)

**Co-Autoren:** Prof. ARCHER, Andrew J. (Loughborough University); Dr. TSELUIKO, Dmitri (Loughborough University); Dr. TOTH, Gyula (Loughborough University); Dr. BANDULASENA, Hemaka C. H. (Loughborough University)

**Vortragende(r):** BOKANYI-TOTH, Agnes (Loughborough University)

**Sitzung Einordnung:** Short Talks

Beitrag ID: 37

Typ: **Talk**

## Tunable shape oscillations in adaptive droplets

*Donnerstag, 7. Dezember 2023 11:00 (25 Minuten)*

Soft materials can undergo irreversible shape changes when driven out of equilibrium [1,2]. When shape changes are triggered by processes at the surface, geometry-dependent feedback can arise. Motivated by the mechanochemical feedback observed in multicellular systems [1,3-5], we study incompressible droplets that adjust their interfacial tensions in response to shape-dependent signals. We derive a minimal set of equations governing the mesoscopic droplet states controlled by just two dimensionless feedback parameters. We find that single adaptive droplets display different classes of excitability arising from a Bogdanov-Takens-Cusp bifurcation, and that interacting droplet pairs exhibit symmetry-breaking and tunable shape oscillations ranging from near-sinusoidal to relaxation-type, which stem from a saddle-node pitchfork bifurcation. Our tractable framework provides a paradigm for how soft active materials respond to shape-dependent signals, and suggests novel modes of self-organisation at the collective scale.

- [1] Erzberger, et al. Nat Phys (2020)
- [2] Salbreux, Jülicher Phys Rev E (2017)
- [3] Dullweber, Erzberger Curr Opin Syst Biol (2023)
- [4] Corson, et al. Science (2017)
- [5] Khait, et al. Cell Rep (2016)

**Hauptautor:** DULLWEBER, Tim (European Molecular Biology Laboratory Heidelberg and Heidelberg Graduate School for Physics)

**Co-Autoren:** Herr KOHEN SAGNER, Ergin (European Molecular Biology Laboratory Heidelberg and Heidelberg University); Herr BELOUSOV, Roman (European Molecular Biology Laboratory Heidelberg); ERZBERGER, Anna (European Molecular Biology Laboratory Heidelberg and Department of Physics and Astronomy, Heidelberg University)

**Vortragende(r):** DULLWEBER, Tim (European Molecular Biology Laboratory Heidelberg and Heidelberg Graduate School for Physics)

**Sitzung Einordnung:** Short Talks

Beitrag ID: 38

Typ: **Poster**

## Directional wicking on topographic micropatterns

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

Directional spreading and wicking of liquid drops on topographic micropatterns are studied on regular arrays of triangular posts breaking the reflection symmetry of the lattice. To test for directional wicking on this class of patterns, we employ heptane drops forming a material contact angle of  $50^\circ$  on Teflon coated samples fabricated using standard photolithography processes. Depending on the density and aspect ratio of the triangular posts, we observe either selective wicking into certain directions, spherical-cap shaped drops with a mobile three-phase contact line, or the formation of drops with a circular or angular pinned three-phase contact line. Drops of the latter class eventually evolve into “sunny-side-up droplets” consisting of a liquid film extending to the initial footprint of the drop immediately after deposition and coexisting with a shrinking cap-shaped drop sitting on the film. The observed directional wicking phenomena can be explained in terms of capillary instabilities at the film edge that govern its mobility at different orientations relative to the micropattern.

**Hauptautoren:** Dr. LIU, Bang-Yan (Department of Chemical Engineering, National Taiwan University, 10617 Taipei, Taiwan); Herr LO, Chi-Chun (Department of Chemical Engineering, National Taiwan University, 10617 Taipei, Taiwan); Frau PENG, Hsuan-Yi (Department of Chemical Engineering, National Taiwan University, 10617 Taipei, Taiwan); Prof. CHEN, Li-Jen (Department of Chemical Engineering, National Taiwan University, 10617 Taipei, Taiwan); BRINKMANN, Martin (Experimentalphysik, Universität des Saarlandes); Prof. SEEMANN, Ralf (Experimentalphysik, Universität des Saarlandes)

**Vortragende(r):** BRINKMANN, Martin (Experimentalphysik, Universität des Saarlandes)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 39

Typ: **Talk**

## Dynamic wetting and dewetting of viscous liquid droplets/films on viscoelastic substrates

*Donnerstag, 7. Dezember 2023 11:50 (25 Minuten)*

Liquid droplets on soft, solid, elastic substrates tend to deform the substrate on which they sit due to the interaction of interfacial and elastic forces. This deformation is the more pronounced the softer the substrate. Our project aims at understanding the mechanisms that determine the resulting morphology of equilibrium droplets.

To study these phenomena, we explore the dewetting of nanoscopic liquid polystyrene (PS) layers from polydimethylsiloxane (PDMS) elastomer substrates with elasticities varying from  $G = 1$  kPa to 2 MPa. The experimental results reveal a strong influence of the PDMS elasticity on the dewetting dynamics. At the late stages of dewetting, we obtain PS droplets sitting on PDMS seemingly surrounded by a “ring” of liquid, non-crosslinked PDMS molecules at the three-phase contact line (TPCL). This ring appears to be more prominent when the PDMS substrate is softer with a larger proportion of non-crosslinked PDMS molecules compared to stiffer PDMS substrates with only a small proportion of non-cross-linked PDMS molecules.

To understand the experimental observations in detail, we are developing certain numerical techniques that allow us to reveal this liquid phase and the corresponding shape of equilibrium droplets for different substrates and adapt a physical model that can explain it.

**Hauptautoren:** REMINI, Khalil (Saarland University); SCHMELLER, Leonie; WAGNER, Barbara (WIAS Berlin); PESCHKA, Dirk (WIAS Berlin); SEEMANN, Ralf (Experimentalphysik, Universität des Saarlandes)

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

**Sitzung Einordnung:** Short Talks



Beitrag ID: 40

Typ: **Poster**

## Not flexible but reactive

*Montag, 4. Dezember 2023 17:50 (20 Minuten)*

Despite its importance in high temperature processes (e.g. welding and coating), the wetting behavior of liquid metals on solid metals (or ceramics) at high temperatures remains poorly understood due to complex physiochemical processes e.g. surface oxidation, Marangoni flows, and interfacial reactions controlling the interfacial properties. Performing experiments above 1000°C requires a strict control of the different phases (gas, liquid, solid) and therefore a complex machinery. It makes it an exciting engineering challenge but also limits the accessibility and interpretation of experimental results. To address these issues, we implemented a combined experimental and numerical study supported by a newly-designed thermo-optical dynamic wetting apparatus, in-situ observation and quenching of liquid/gas interfaces by a confocal laser scanning microscope, molecular dynamics, and computational fluid dynamics simulations. Our study comprehensively explores the high-temperature wetting behaviors across various systems, including non-reactive Al/Al<sub>2</sub>O<sub>3</sub>, dissolutive Cu/Ni and reactive Al/Ni systems. Key aspects investigated involve the evolution of oxides and Marangoni flow at liquid/gas interfaces, physiochemical interactions at liquid/solid interfaces and their impact on spreading dynamics.

**Hauptautor:** SUN, Youqing (KU Leuven)

**Vortragende(r):** SUN, Youqing (KU Leuven)

**Sitzung Einordnung:** Poster Session

Beitrag ID: 41

Typ: Talk

## Adaptive Wetting and Actuating Devices based on Conducting Polymer Materials

*Dienstag, 5. Dezember 2023 17:25 (25 Minuten)*

Conducting polymers (CPs) are discussed in a huge variety of electronic devices including organic field effect transistors, batteries, actuators and (bio)electronic sensors. Compared to other conducting materials, CPs are light-weight, low cost, non-toxic, flexible and allow easy processing, low voltage operation (around 1 Volt) and low power consumption.

Here, poly(3-hexylthiophene) (P3HT) and poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) are presented as work-horses of our team due to their high conductivities and electrochromism which can be accessed by tailor-made doping. The doping states of these semiconductors can be controlled by electrochemical or chemical doping. A former study in our team showed that for P3HT an increase in conductivity over 6 orders of magnitude can be obtained as function of increasing electrochemical doping potential, giving maximum conductivities as high as 200 S/cm.<sup>1</sup> Currently, we are working on using this electrochemical doping strategy to induce changes in chemical and physical properties of P3HT and PEDOT:PSS. Particularly interesting for the priority program SPP-2171 is our finding that also the wettability and the water uptake (sorption) dramatically change as function of the doping level.

Due to the fact that PEDOT:PSS is a mixed conductor, it also strongly depends on the relative humidity (r.H.) which makes it possible to build humidity-responsive bilayer actuators.<sup>2</sup> The curvature of such humidity-triggered actuators can be explained by a combined study of rheology including wetting and water uptake studies

### References

- (1) D. Neusser, C. Malacrida, M. Kern, Y. Gross, J. van Slageren, S. Ludwigs, *Chem. Mater.*, **2020**, 32, 6003.
- (2) C. Dingler, H. Müller, M. Wieland, D. Fauser, H. Steeb, S. Ludwigs, *Adv. Mater.*, **2021**, 33, 2007982.

**Hauptautoren:** LI, Jie (MIB, University Stuttgart); LU, Junqi (Institute of Polymer Chemistry (IPOC), University of Stuttgart); LUDWIGS, Sabine (IPOC, University of Stuttgart); STEEB, Holger (MIB, University Stuttgart)

**Vortragende:** LI, Jie (MIB, University Stuttgart); LU, Junqi (Institute of Polymer Chemistry (IPOC), University of Stuttgart)

**Sitzung Einordnung:** Short Talks

Beitrag ID: 42

Typ: **Poster**

## Growing biofilms on elastic substrates

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

In this study, we aim to investigate the influence of substrate properties on biofilm spreading using a simplified model tailored to elastic substrates. The contact angle plays a key role in biofilm spreading and is related to the spreading velocity. To facilitate our mesoscale analysis, we use a model of wetting energy as a function of film height, denoted  $f(h)$ . In a departure from the conventional view of rigid solid substrates, our research aims to uncover the profound influence of mechanical substrate properties on biofilm behavior. By manipulating substrate compliance, covering the spectrum from the solid state ( $s < 10$ ) to the elastic range ( $10 < s < 1 \times 10^5$ ), while keeping the values of surface tension ( $\gamma_h = 0.1$ ) and droplet volume ( $V = 1 \times 10^5$ ) constant, our study focuses on the comprehensive evaluation of critical parameters, including wettability, biofilm growth production, and substrate softness.

**Hauptautoren:** PIETZ, Anthony Lennard; JOHN, Karin; THIELE, Uwe

**Vortragende(r):** PIETZ, Anthony Lennard

**Sitzung Einordnung:** Poster Session

Beitrag ID: 43

Typ: **Talk**

## Gradient dynamics approach to chemically reacting sessile liquid drops

*Dienstag, 5. Dezember 2023 15:40 (25 Minuten)*

We present a gradient dynamics approach to thin-film models with chemical reactions. In particular, we treat sessile liquid drops that are covered by two species of autocatalytically reacting surfactants. The gradient dynamics form is then broken by introducing external chemostats such that the system is rendered active. We analyze the resulting dynamics using numerical continuation and time simulations and find, inter alia, different modes of drop oscillation (symmetric, anti-symmetric, asymmetric with respect to parity) and self-propelled drops.

**Hauptautoren:** VOSS, Florian Alexander; THIELE, Uwe

**Vortragende(r):** VOSS, Florian Alexander

**Sitzung Einordnung:** Short Talks

Beitrag ID: 45

Typ: **Keynote**

## Self-propulsion of floating objects driven by the Marangoni flow induced by the presence of multiple species

*Dienstag, 5. Dezember 2023 09:00 (20 Minuten)*

Floating objects that releases volatile surface active material shows self-propulsion by generating the Marangon flow around the object. Typical example is a camphor particle on a water surface, which shows self-propulsion by the spontaneous fore-aft and/or rotational symmetry breaking around the particle. Interestingly, such surface active material also induces effective interaction between particles that can be nonreciprocal; i.e., the broken action-reaction laws. In such a case with the multiple type of objects, the different types of objects experiences nonreciprocal interaction, and they creates self-propelling pair owing to the unbalanced effective force. Here, we show several systems of floating objects with multiple species, and especially talk about the system with binary droplets, PFD and decane droplets, on water. The system showed self-propulsion, as well as the repetitive activity that resembles eruptive motion. We discuss the behavior in terms of the presence of duplex films on the water surface.

**Reference:**

[1] Yutaka Sumino, Ryo Yamashita, Kazuki Miyaji, Hiroaki Ishikawa, Maho Otani, Daigo Yamamoto, Erika Okita, Yasunao Okamoto, Marie Pierre Krafft, Kenichi Yoshikawa and Akihisa Shioi, "Droplet duos on water display pairing, autonomous motion, and periodic eruption", *Sci. Rep.* 13,12377-1-10 (2023).

[2] Hiroaki Ishikawa, Yuki Koyano, Hiroyuki Kitahata, and Yutaka Sumino "Pairing-induced motion of source and inert particles driven by surface tension", *Phys. Rev. E.* 106,024604-1-11 (2022).

**Hauptautoren:** SUMINO, Yutaka; ISHIKAWA, Hiroaki; OTANI, Maho; YAMAMOTO, Daigo; OKITA, Erika; OKAMOTO, Yasunao; KRAFFT, Marie Pierre; YOSHIKAWA, Kenichi; SHIOI, Akihisa

**Vortragende(r):** SUMINO, Yutaka

**Sitzung Einordnung:** Keynote

Beitrag ID: 46

Typ: **Keynote**

## Renewable Energy Networks —a playground for Applied Theoretical Physics

*Mittwoch, 6. Dezember 2023 18:30 (20 Minuten)*

In view of critical CO<sub>2</sub> emissions and depleting conventional resources, a transformation towards a sustainable energy system is needed. Applied Theoretical Physics and the Physics of Complex Networks are able to contribute to the solution of this grand challenge. We discuss a simple network model, which describes a future European electricity system with a high share of wind and solar power generation. The weather acts as the fluctuating driving force. Weather data covering multiple years are converted into prospective wind and solar power generation with good spatial and temporal resolution. The weather-driven network modelling represents a direct approach to obtain fundamental estimates on the required backup infrastructure of highly renewable large-scale energy systems. Estimates on the required amount of conventional backup power plants, transmission lines and storage will be given. The optimization of energy system costs is addressed, leading to new design concepts like the optimal heterogeneity and the benefit of cooperation. Related to diffusion processes on networks, flow tracing algorithms are described, which help to clarify how the resulting costs are shared in a fair manner. An extended outlook about current research on the coupling of the different energy sectors, the techno-economical design and socio-political implementation of decarbonization roadmaps into the future as well as the impact of climate change will be given at the end.

**Hauptautor:** GREINER, Martin

**Vortragende(r):** GREINER, Martin

**Sitzung Einordnung:** Evening Talk

Beitrag ID: 47

Typ: **Talk**

## Volatile binary mixtures on polymer brushes

*Dienstag, 5. Dezember 2023 10:10 (25 Minuten)*

We present a mesoscopic thin-film model in gradient dynamics form for binary liquid mixtures on brush-covered substrates incorporating volatility in a narrow gap. Thereby, we expand models established in [1, 3, 4], for one substance by incorporating a second substance present in each of the three bulk phases - liquid, brush and gas [1, 2]. We discuss the different contributions to the free energy, thereby employing Flory-Huggins theory of mixing for the condensed phases and assuming ideal gases for the vapor phase. Interface energies are modeled as linear interpolations of known limiting cases. The resulting six-field model is then analyzed with numerical time simulations showing results with a focus on lateral concentration gradients, notably at the contact line.

[1] S. Hartmann, C. Diddens, M. Jalaal, and U. Thiele. Sessile drop evaporation in a gap: crossover between diffusion-limited and phase transition-limited regime. June 2022.

[2] L. A. Smook, G. C. R. van Eck, and S. de Beer. Friends, foes, and favorites: Relative interactions determine how polymer brushes absorb vapors of binary solvents. *Macromolecules*, 53(24):10898–10906, dec 2020. doi: 10.1021/acs.macromol.0c02228.

[3] U. Thiele and S. Hartmann. Gradient dynamics model for drops spreading on polymer brushes. *The European Physical Journal Special Topics*, 229(10):1819–1832, sep 2020. doi: 10.1140/epjst/e2020-900231-2.

[4] Ozlem Kap, S. Hartmann, H. Hoek, S. de Beer, I. Siretanu, U. Thiele, and F. Mugele. Nonequilibrium configurations of swelling polymer brush layers induced by spreading drops of weakly volatile oil. *The Journal of Chemical Physics*, 158(17), 2023. doi: 10.1063/5.0146779

**Hauptautoren:** DIEKMANN, Jan; THIELE, Uwe

**Vortragende(r):** DIEKMANN, Jan

**Sitzung Einordnung:** Short Talks

Beitrag ID: 48

Typ: **Talk**

## Percolation in Networks of Liquid Diodes

*Mittwoch, 6. Dezember 2023 10:10 (25 Minuten)*

Liquid diodes are surface structures that facilitate the spontaneous flow of liquids in a specific direction. In nature, they are used to increase water collection and uptake, reproduction, and feeding. However, large networks with directional properties are exceptional and are typically limited up to a few centimeters. Here, we simulate, design, and 3D print liquid diode networks consisting of hundreds of unit cells. We provide structural and wettability guidelines for directional transport of liquids through these networks and introduce percolation theory in order to identify the threshold between a connected network, which allows fluid to reach specific points, and a disconnected network. By constructing well-defined networks with uni- and bidirectional pathways, we experimentally demonstrate the applicability of models describing isotropically directed percolation. We accurately predict the network permeability and the liquid final state. These guidelines are highly promising for the development of structures for spontaneous, yet predictable, directional liquid transport.

**Hauptautoren:** PINCHASIK, Bat-El; SAMMARTINO, Camilla; SHOKEF, Yair

**Vortragende(r):** SAMMARTINO, Camilla

**Sitzung Einordnung:** Short Talks



Beitrag ID: 49

Typ: **Keynote**

## Elastohydrodynamic relaxation of porous films and slender fibers

*Mittwoch, 6. Dezember 2023 14:30 (20 Minuten)*

The deformation of soft and flexible objects is a common elastohydrodynamic scenario. In this presentation, we consider deformable surfaces and flexible fibers subjected to hydrodynamic and capillary stresses, and the resulting dynamical approaches to equilibrium. First, we consider a rigid object approaching a poroelastic material in a viscous fluid, for which hydrodynamic stresses arise in the lubricated contact region and deform the soft material. The elastic deformation modifies in turn the flow, hence generating a soft-lubrication coupling. As revealed by our analytic model making use of linear poroelastic theory, the effect of porosity in this scenario is essentially to divide the response into compressible and incompressible parts, with a diffusive temporal crossover separating the two purely elastic responses. Second, we consider a slender fiber prepared in a microfluidic chip, subject to capillary stresses at the surface of a confined and driven droplet. In general, the equilibria for these types of liquid-fiber systems depend on surface tension and the bending modulus of the deformable object. Indeed, a plethora of self-assembled structures including coiled droplets, bundled hair and capillary origami have been observed elsewhere. If these equilibria are well described in the literature, the dynamic equilibration path in surrounding hydrodynamic flow has been less reported. Our system provides a model visco-elasto-capillary relaxation context, starting from a model non-equilibrium state. We thus observe and describe theoretically the dynamic retraction of a slender fiber into a moving droplet.

**Hauptautor:** MCGRAW, Joshua

**Vortragende(r):** MCGRAW, Joshua

**Sitzung Einordnung:** Keynote

Beitrag ID: 50

Typ: **Keynote**

## Why I love surfactants

*Mittwoch, 6. Dezember 2023 09:00 (20 Minuten)*

Surfactants are very familiar molecules. They exist in nature and are widely used in industry as well as in our daily lives. We know that they accumulate at interfaces, that they modify interfacial energy, that they can self-assemble and that they can interact via electrostatic or hydrophobic interactions. Extremely familiar and well characterized, in this talk I would like to how also amazing they remain, and how tiny quantities of these molecules enable remarkable behaviours including 1) self-propulsion of water on bare glass; 2) light-driven microfluidic operations (transport, mixing); 3) liquid marble actuation and anti-Marangoni transport (slide effect); 4) coffee-ring diagnostics; 5) reconfigurable colloidal assembly (dissipative and living crystals); 6) controlled particle deposition with various degrees of complexity (from monocrystals to polycrystalline disks and “irises”, from single-component assemblies to crystal alloys).

**Hauptautor:** BAIGL, Damien**Vortragende(r):** BAIGL, Damien**Sitzung Einordnung:** Keynote

Beitrag ID: 51

Typ: **Keynote**

# Current problems in kinetics of wetting and spreading

*Montag, 4. Dezember 2023 14:00 (20 Minuten)*

There has been a substantial increase in the number of publications in the field of wetting and spreading since 2010 [1]. This increase in the rate of publications can be attributed to the broader application of wetting phenomena in new areas.

The current state of the art in the field of wetting and spreading will be presented. Selected topics in the field are as follows: (i) Contact angle hysteresis on smooth homogeneous solid surfaces via disjoining/conjoining pressure. It is shown that the hysteresis contact angles can be calculated via disjoining/conjoining pressure. The theory indicates that the equilibrium contact angle is closer to a static receding contact angle than to a static advancing contact angle. (ii) The wetting of deformable substrates, which is caused by surface forces action in the vicinity of the apparent three-phase contact line, leading to a deformation on the substrate. (iii) The kinetics of wetting and spreading of non-Newtonian liquid (blood) over porous substrates. It is showed that in spite of the enormous complexity of blood, the spreading over porous substrate can be described using a relatively simple model: a power low-shear-thinning non-Newtonian liquid. (iv) The kinetics of spreading of surfactant solutions. In this part, new results related to various surfactant solution mixtures (synergy and crystallization) are discussed, which shows some possible direction for the future revealing of superspreading phenomena. (v) The kinetics of spreading of surfactant solutions over porous materials including hair and biofilms.

The importance of the topic will be presented and fundamental problems to be solved identified.

## References

[1] O. Arjmandi-Tash, N. M. Kovalchuk, A. Trybala, I. V. Kuchin, V. Starov, *Langmuir*, 2017, 33, 4367–4385.

**Hauptautoren:** TRYBALA, Anna; TAFIREYI, Wellington

**Vortragende(r):** TRYBALA, Anna

**Sitzung Einordnung:** Keynote

Beitrag ID: 52

Typ: **Keynote**

## Three problems involving ternary fluid systems

*Donnerstag, 7. Dezember 2023 09:00 (20 Minuten)*

Ternary fluid systems often require an extra layer of complexity in describing the surface morphologies and interfacial flows. On the other hand, the physics and dynamics of such systems are of special interests for a variety of practical applications, ranging from microfluidics to oil recovery, combustion engines and lubricated surfaces. In this talk I will discuss our numerical and experimental results in relation to three of such applications, namely double emulsion formation in microfluidic flow-focusing devices; drop impact between immiscible liquid droplets; and the drop and ridge dynamics on Slippery Liquid Infused Porous Surfaces (SLIPS).

**Hauptautor:** SEMPREBON, Ciro

**Vortragende(r):** SEMPREBON, Ciro

**Sitzung Einordnung:** Keynote

Beitrag ID: 53

Typ: **Poster**

## Wetting fronts underneath impacting drops on oily substrates

*Montag, 4. Dezember 2023 18:10 (20 Minuten)*

When a droplet impacts on a plane solid covered by an oil layer of few micrometers thickness, an air layer is entrained. The moment of rupture is determined by the thickness profile and the presence of impurities in the experimental configuration. A central dimple in the droplet is surrounded by a broad plateau of only slowly varying thickness with radius. After initiation of contact, the thin air film is expelled by a wetting front, which surprisingly develops a fingering instability in some cases. We study the propagation of the wetting fronts from high-speed interferometric videos. We expect that both oil layer and droplet properties affect the contact spreading, and the air layer thickness should have a minor effect. Apparently, the oil layer has crucial impact on the contact line velocity.

**Hauptautoren:** MORADIMEHR, Shiva; HARTH, Kirsten

**Vortragende(r):** MORADIMEHR, Shiva

**Sitzung Einordnung:** Poster Session

Beitrag ID: 54

Typ: Talk

## On Demand Modulation of Adhesion of Lipid Vesicles and Biological Cells on Switchable Substrates

Mittwoch, 6. Dezember 2023 17:05 (20 Minuten)

Wetting and adhesion of lipid vesicles and biological cells are distinct from that of Newtonian fluid, because of their viscoelasticity. The use of switchable substrates based on polymer brushes and hydrogels offers a unique advantage for the adjustment of interfacial interactions on demand.

In the first of my talk, I will introduce our collaborative activities with Müller group (Göttingen) within the framework of SPP2171. Here, we utilized stimulus responsive polymer brushes whose conformation can be reversibly switched by the presence of metal ions. The change in the polymer chain conformation is accompanied by the modulation of interfacial viscoelasticity and interfacial potentials [1]. We monitored the global shape of vesicles using confocal microscopy and the local height profile near the surface using micro-interferometry [2]. In addition to the regulation of vesicle shape and hence adhesion free energy under static conditions, we also monitored the change in vesicle shape caused by the dynamic change in brush conformation in situ.

In the second part, I will extend the topic and show you some examples that a very similar approach can be taken to mechanically stimulate biological cells by the use of switchable hydrogels [3].

### References

[1] aA. Yamamoto, T. Ikarashi, T. Fukuma, R. Suzuki, M. Nakahata, K. Miyata, M. Tanaka, *Nanoscale Advances* 2022, 4, 5027-5036; bA. Yamamoto, K. Hayashi, A. Sumiya, F. Weissenfeld, S. Hinatsu, W. Abuillan, M. Nakahata, M. Tanaka, *Frontiers in Soft Matter* 2022, 2, 959542.

[2] F. Weissenfeld, L. Wesenberg, M. Nakahata, M. Müller, M. Tanaka, *Soft Matter* 2023, 19, 2491-2504.

[3] aM. Hippler, K. Weißenbruch, K. Richler, E. D. Lemma, M. Nakahata, B. Richter, C. Barner-Kowollik, Y. Takashima, A. Harada, E. Blasco, M. Wegener, M. Tanaka, M. Bastmeyer, *Science Advances* 2020, 6, eabc2648; bM. Hörning, M. Nakahata, P. Linke, A. Yamamoto, M. Veschgini, S. Kaufmann, Y. Takashima, A. Harada, M. Tanaka, *Scientific Reports* 2017, 7, 7660; cV. Frank, S. Kaufmann, R. Wright, P. Horn, H. Y. Yoshikawa, P. Wuchter, J. Madsen, A. L. Lewis, S. P. Armes, A. D. Ho, M. Tanaka, *Scientific Reports* 2016, 6, 24264.

**Hauptautor:** TANAKA, Motomu

**Vortragende(r):** TANAKA, Motomu

**Sitzung Einordnung:** Short Talks