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Liquids on switchable pre-structured substrates – from microscopic to mesoscopic models

Project Description

In this project we will study the static and dynamic properties of a simple liquid on *a switchable pre-structured substrate* from a numerical/theoretical perspective in close contact to the both experimental and theoretical projects of the SPP. Whereas the wetting behavior on homogeneous and pre-structured substrates is well-understood, we aim to obtain a thorough understanding of the resulting *non-equilibrium* effects upon switching, involving new time-scales as in the case of periodic switching. Prominent effects are expected, e.g., for the wetting of close-by hydrophilic stripes, involving liquid bulge as well as bridge configurations.

For a comprehensive understanding of the system in question we are convinced that an analysis of different length- and time-scales is of utmost importance. For example, in order to take into account the switching process itself, a microscopic analysis is required and, indeed, we will explicitly study the switching of photoactive molecules via Molecular Dynamics simulations (MD) and its impact on the liquid. In contrast, to study the long-time behavior to new equilibrium states, a continuum perspective will be most appropriate where, e.g., the dynamical behavior and arising instabilities can best be analyzed. For specific questions, and fully related to the scientific expertise of the two PIs, we will combine force field and lattice gas simulations, on the one hand, and mesoscopic thin film models studying the gradient dynamics on interface Hamiltonians, on the other hand.

In order to have a quantitative matching among these approaches, we employ specific multiscale bridging techniques to perform the parameter passing to the mesoscopic thin film approach, i.e. the estimation of the tension and the wetting potential. For MD simulations, the information can be directly obtained from the calculation of appropriate virials whereas for the case of a LGM, a bridging microscopic Density Functional Theory will be employed, as developed in a recent collaboration of both PIs. The matched hierarchy of models shall allow us to quantitatively understand crucial aspects of non-equilibrium deposition and rearrangement processes of the molecules across several length and time scales.

During this three year period we aim (i) to gain full experience with the relevant theoretical tools, (ii) to obtain a good physical understanding of non-equilibrium effects upon switching, and (iii) to apply these results, in close collaboration with the corresponding experimental groups of the SPP, to the specific interaction parameters of their experiments (e.g., for given pre-structuring and contact angles).

1 State of the art and preliminary work

1.1 State of the art

Many coating and surface growth processes where a solid substrate is covered by homogeneous or structured layers of the same or other materials combine deposition and redistribution stages that might occur successively or in parallel. Prominent examples are various homo- and heteroepitaxial surface growth processes where the redistribution of material on the substrate occurs through diffusion of deposited atoms or molecules on the surface of the substrate [1, 2]. Other examples are e.g., dip-coating and related processes

where a liquid is transferred from a bath or other reservoir onto the substrate [3–5]. These examples all involve a wet stage where hydrodynamic flows caused by external forces, wettability, and capillarity are important for the redistribution of the material.

Many of the studied systems involve homogeneous substrates. However, over the past decades, effects of heterogeneous substrates on the wetting behavior have been extensively investigated experimentally and theoretically to achieve determined liquid structures or to control the dynamic self-assembly of organic molecules that show a liquid-like behavior. Thereby, the pre-structuring can be of topographical type [6, 7], purely chemical, i.e. affecting the local wetting properties [8–13], or a combination of both [14]. Experimental examples include macroscopic experiments with water on chemically heterogeneous substrates [15], experiments in dip-coating [16] and Langmuir-Blodgett geometries [17], dewetting of thin silicon films on nano-patterns formed by electron beam lithography [18] or deposition experiments with organic molecules on silicon oxide substrates with gold stripes [19, 20], to name but a few. In the latter case the emerging structures typically depend on the deposition rate and thus have to be described as the result of a non-equilibrium process.

Theoretically, the behavior of the molecules can be modeled on an atomistic level by MD simulations [21] or on a more coarse grained level by MC simulations of a LGM [22, 23]. The latter may be also formulated in a *Kinetic Monte Carlo* (KMC) framework, based on estimated rate constants [24]. A combination of topographical and chemical pre-patterns is accounted for in [14], where atomistic KMC simulations are conducted. In general, LGM can be used to characterize the different nucleation processes, the generation of self-assembled structures as well as the occurrence of instabilities for particles on pre-structured substrates [Lie12] [25]. Another application is the understanding of a liquid bridge between plates [26, 27]. This analysis can be extended to the case of flow, i.e. micro- or nanofluidics, showing distinct microscopic effects in the nanoregime which are not present in macroscopic hydrodynamic equations [24].

In the LGM one has energy scales for the interaction between particles ϵ_{pp} and between particles of the deposited liquid and the substrate ϵ_{ps} (or different substrates). Recently it has been shown that by appropriate choice of nearest-, second-nearest, and third-nearest neighbor interactions the resulting droplets on the substrate display a hemispherical shape [28], thus strongly reducing the undesired impact of the underlying lattice.

Whereas KMC and MD simulations can incorporate more details of the specific interactions between the deposited molecules as well as between molecules and substrate, *continuum models* are able to address much larger length and time scales. Further, with continuum models one may (semi-)analytically analyze instabilities of the liquid structures and provide experimentalists with general results. Static liquid structures on a substrate with a chemical stripe-like pre-pattern and their morphological changes are investigated in [29–31] based on the minimization of effective interface energies. From these studies, in agreement with simulations of a LGM, a large range of morphologies can be observed for these pre-patterns. In [30], a spatially varying effective interface potential is employed to model a pre-structure patch in two dimensions, the investigation in [29] is conducted for three-dimensional liquid structures on a single pre-structure stripe and two adjacent pre-structure stripes. The dynamics of a liquid on a pre-structured substrate is investigated in [8, 32, 33] by direct numerical simulations of thin-film (TF) equations with spatially varying disjoining pressures. Similar equations are considered in [34, 35], where bifurcation diagrams for static ridge-like states are determined and their transversal stability is analyzed. However, the effects of the switchable pre-structured substrates on the dynamical behavior of liquid drops is not understood to a large extend.

Given the advantages and disadvantages of the different theoretical and numerical methods, it is evident that a *mapping* between the methods is of great interest. An important input for any mesoscopic hydrodynamic model are the parameters and expressions that characterize capillarity and wettability. Namely, these are the interfacial tensions and the film height-dependent wetting (or binding) potential, respectively. The precise form of the wetting potential determines whether or not the liquid wets the surface and is directly related to the Derjaguin (or disjoining) pressure that determines (beside the Laplace pressure) the pressure gradient that drives the dynamics in a liquid film or drop. Within lattice (dynamical) density functional theory (lattice (D)DFT) the lattice gas model can be mapped on site probabilities which can be interpreted

as the probability to observe a particle at that location when averaging over many LGM simulations. The key advantage of the probability distribution is the availability of a free energy functional. Within a mean field approach it is possible to map the LGM on a set of rate equations for these site probabilities and to express these equations as Cahn-Hilliard type equations which are typical for a lattice DDFT approach [36]. A microscopic density functional theory (DFT) as well as continuum DFT based methods for calculating the wetting potential allowing to relate its form to the nature of the molecular interactions in the system was discussed in [28,37]. An alternative approach via a MD simulations is described in [38,39]. The continuous DFT used in [37] includes the influence of the layering of molecules close to interfaces and the resulting oscillatory density profiles. The calculated *static* drop shapes are shown to be in quite good agreement with drop profiles determined directly from the microscopic DFT. However, some details of the extraction of wetting potentials are still tricky and there remain some open questions. In particular, an important question is the extraction of *transport coefficients* from microscopic simulations (as MD or Kinetic Monte Carlo (MC) simulations) to come to a fully *quantitative mapping* of microscopic and mesoscopic theories not only for the static but also for the *dynamic* behavior.

1.2 Preliminary work

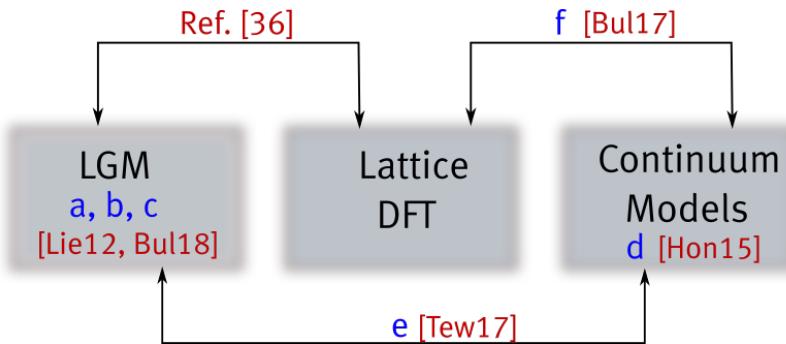


Figure 1: A schematic overview of multiscale modeling for liquids on prepatterned substrates conducted by both PIs. The preliminary work labeled with a-f is described below in more detail.

The research project relies on complementary expertise provided by the two project partners, building upon a long-term collaboration. The summary of recent results is described below. In particular, we have gained a broad expertise on *multiscale theoretical modeling* ranging from microscopic level to mesoscopic continuum models of self-organization processes (see Fig. 1). A combined coarse-grained lattice type and continuous description was developed in order to understand the structure formation, transport processes and stability of liquids and organic molecules showing liquid-like behavior on prepatterned substrates [40]. Whereas the atomistic perspective was handled via LGM simulations [Lie12,Wan16, Bul18], the mesoscopic methods range from (lattice) DDFT to the use of an interface Hamiltonian in mesoscopic thin film hydrodynamics approaches [Hon15, Wil15], based on the solution of partial differential equations via path continuation [Eng19] and time simulations. While a qualitative agreement between microscale and mesoscale modelling approaches was shown in [Tew17], a first step towards a quantitative mapping between these different scales is achieved via parameter passing methods, such as extracting wetting potentials via a novel numerical Nudged Elastic Band approach [Bul17]. To achieve large time and length scales, newly developed grid-based numerical methods are used.

After this general overview we now present some of our preliminary work in more detail.

a: LGM to describe bulge formation As a key application to use LGM simulations in the context of structure formation of vapor deposited molecules, the growth on stripes as a function of particle-particle interaction was studied [Lie12]. As shown in Fig.2 three growth regimes can be identified (homogeneous coverage of stripe, elliptic and highly symmetric bulges, irregular nucleation, triggered by the presence of gold stripes). Experimentally, these scenarios have been observed in the group of L.F. Chi when classifying the structure formation of several organic molecules.

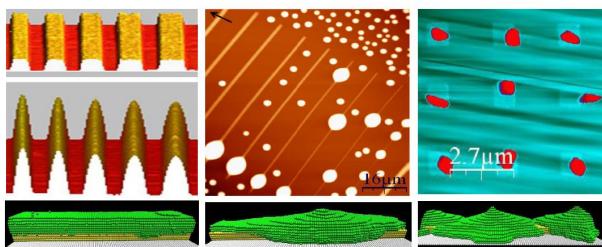


Figure 2: Upper row Structure formation on gold stripes for three different organic molecules (NPB, DTCDQA and PTCDA). Lower row: Results of LGM simulations with an increasing particle-particle interaction (from left to right) [Lie12].

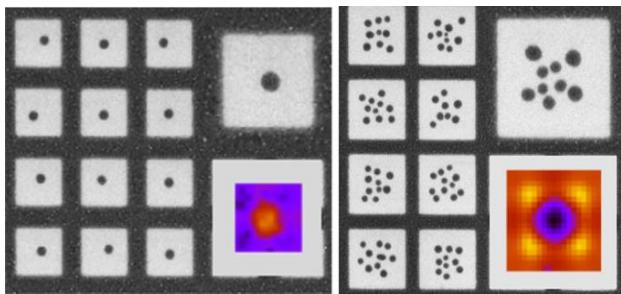


Figure 3: Comparison of the experimentally observed clusters for different grid sizes. Included is the size distribution of the clusters, as observed from lattice gas model simulations. Depending on the grid size one observes a specific number of clusters per cell. Interestingly, a high nucleation and position order is observed in the left case [Wan16].

b: Understanding Nucleation Control on pre-structured substrates As a further application of using a LGM we have studied the cluster growth on substrates which are pre-structured with regular gold grids [Wan16, Bul16]. In contrast to previous work, nucleation does not take place at the position of the grid lines. Instead, the grid renders the concentration of adsorbed molecules position-dependent and thus triggers cluster formation at specific positions. This gives rise to boundary-induced nucleation and position control. Experimentally, for appropriate combinations of grid size and deposition flux one can achieve a perfect nucleation control, namely, induce exactly one nucleus per cell. The method is very versatile and can be used for very different organic molecules. Furthermore, the nuclei are centered close to the middle of the cell. This can be perfectly reproduced by LGM simulations; see Fig. 3.

Actually, it is possible to derive specific scaling laws [Bul18] and to rationalize them via analytical calculations. In particular, this is a clear-cut example where the scaling works for all length scales so that the simulation data, obtained on the nanoscale, can be quantitatively extrapolated to the experimentally relevant microscale.

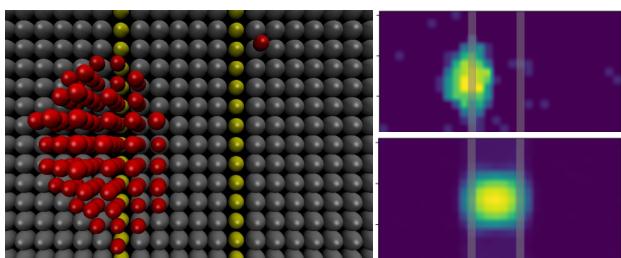


Figure 4: Left: Snapshot of the initial configuration for the free energy calculation of a droplet on a pre-structured substrates, containing two close-by stripes which attract the particles. Right: The density distributions of all configurations without long MC simulations where the center of mass is either on the left stripe (*bulge configuration*) or exactly in the middle between both stripes (*bridge configuration*), respectively.

c: Studying metastable states for close-by stripes: free energy calculations When studying the structure formation on pre-structured substrates with close-by stripes, it has been experimentally observed that two topologically different (meta-)stable states exist [41]. Beyond the bulge formation on a stripe (*bulge configuration*), discussed above, the particles may agglomerate in-between both stripes (*bridge configuration*).

Indeed, based on the minimization of expressions for interfacial free energies, both types of states could be described [29]. We have started to elucidate this behavior via LGM simulations (recent Master thesis of

Leon Topp in the Heuer group). Depending on the choice of the key parameters (e.g. number of particles N , distance d and width of stripes) either configuration may be the stable one. The density map for both (meta-)stable configurations is shown in Fig.4(right).

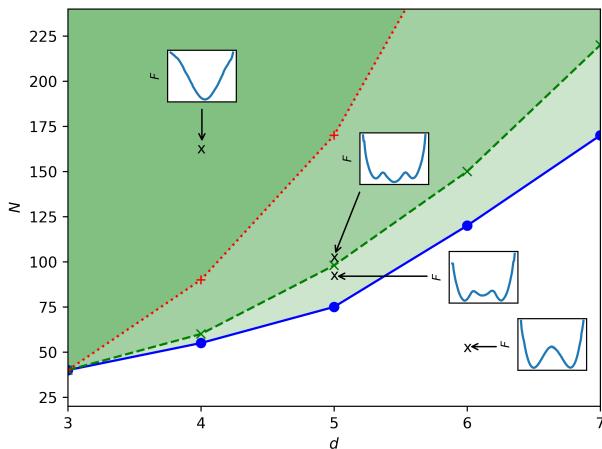


Figure 5: A phase diagram in dependence of the number of particles and the distance of two adjacent stripes. Regimes of different behavior with respect to the occurrence of bulge and bridge configurations are shown. Of particular relevant for the present proposal is the broken green line where both configurations have identical free energies. A closer analysis shows that the bridge configurations are mainly stabilized by entropic contributions.

Of primary importance is the free energy in dependence of the position of the center of mass of the droplet. Using Markov State Modelling [42] it is indeed possible to extract this information from the MC simulations, even in case of relatively high barriers where overall equilibration is hardly possible. A phase diagram is shown in Fig.5.

Most importantly, there is a parameter regime where both states have a similar probability. As a consequence, a minor change of, e.g., the energetic parameters of the model can transform the metastable configuration in a stable configuration and vice versa. In general, the bulge configuration is stable for large distances d and/or small number of particles N . Finally, going beyond the general free-energy calculations, a simulation approach allows one to determine the individual energetic and entropic contributions. For example, it turns out that the bridge state is largely stabilized by entropic effects.

d: Mesoscopic continuum thin film description While the microscopic analysis of the structure formation, described in [Lie12] mainly reflects nanoscopic properties of the molecules, a deeper understanding of the redistribution stage of deposition experiments can be obtained employing a mesoscopic continuum model. Assuming that the slope of the free surface is everywhere small (thin-film or long-wave approximation [43], cf. [Wil15]), an asymptotic model for the dynamics of the height profile of a liquid film is derived from the basic hydrodynamic equations. The gold prepattern is introduced as a chemical heterogeneity that affects the wettability and is incorporated as a spatially modulated wetting potential [Hon15]. It represents the mesoscopic way to define different equilibrium contact angles on distinct areas. Within this model, the linear stability of transversally invariant ridges located on the more wettable parts of a stripe pattern was analyzed using numerical path continuation and time simulations. Note that on homogeneous substrate, such ridge solutions are always unstable w.r.t. transversal (i.e., Plateau-Rayleigh) instabilities [34].

However, the prepattern can *stabilize* the structure in certain regions of parameters like the prepattern strength, prepattern size and the liquid volume in the ridge. We have focused on the regime where the ridge is transversally unstable. It was found that there exist two qualitatively different instability modes that lead (i) at large ridge volume to the formation of bulges that spill from the more wettable stripes onto the less wettable bare substrate and (ii) at small ridge volume to the formation of small droplets located on the more wettable stripes. These instabilities can be identified as a Plateau-Rayleigh instability and a surface instability (as in the spinodal dewetting of a thin film on homogeneous substrate), respectively. Further, the role of the transversally invariant ridge states in the course of the fully nonlinear time evolution was investigated. It was found that the unstable ridge state as well as other unstable states (e.g., multidrop states)

represent important transients that structure the time evolution where they result in prominent plateaus in the free energy (Fig. 6). Indeed, each plateau represents one of the unstable steady state. This observation is also important for other gradient dynamics systems as it indicates how important it is to understand the *complete* solution structure of a system in order to control its time evolution. It is further to expect that the unstable steady states are the ones that are most easily stabilized through imposed controls, e.g., spatio-temporal patterning. Moreover, the sequence of unstable states (and corresponding energy plateaus) observed in the

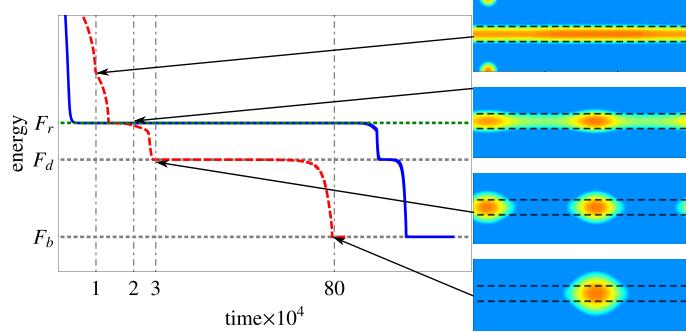


Figure 6: Time series of the free energy during the direct time simulation of the thin-film equation for transport by surface diffusion (solid blue line) and by convection (dashed red line) are shown with the snapshots that correspond to the various energy plateaus: The ridge becomes unstable w.r.t. transversal instability and evolves into bulges that also cover part of the less wettable stripe [Hon15].

time simulation only weakly depends on the transport process, that mainly influences the ratio of the time scales of the different process phases (cf. in Fig. 6 solid blue and dashed red lines for the transport by surface diffusion and by convection, respectively). That is, we have found that the different experimentally observed equilibrium morphologies result from different balances of interface and wetting energies and not from the different transport mechanisms that dominate either in the liquid or in the solid state.

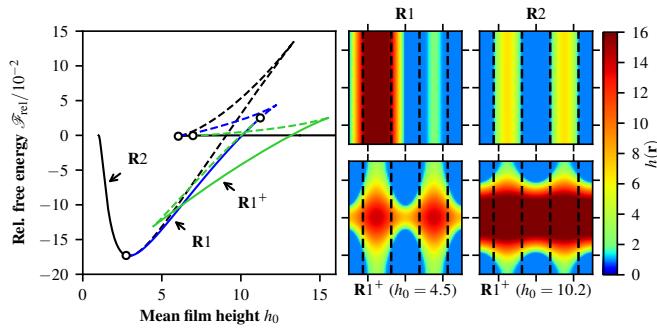


Figure 7: Steady state solutions of the thin-film equation for partially wetting liquids on a heterogeneous substrate with two hydrophilic stripes. (Left) the bifurcation diagram in dependence of the mean film height employing again the energy relative to a flat film solution. Linearly stable and unstable solutions are indicated by solid and dashed lines, respectively. (Right) selected corresponding solution profiles [Eng19].

The unstable states cannot be reached by direct numerics, however it becomes possible within so-called *path following methods* that can efficiently track the entire solution structure and its stability. In [Hon15, Tew17], the path continuation was implemented for one-dimensional steady state solutions of the thin film equation. However, efficient *two-dimensional* continuation tools were developed recently and successfully applied to thin film equation and related problems (see e.g., [44, 45], [Eng19]). One example of a two-dimensional path continuation is shown in Fig. 7. There, a bifurcation diagram showing steady state solutions of the thin-film equation for partially wetting liquids on a prepatterned substrate with two static hydrophilic stripes is depicted together with corresponding stable and unstable solution profiles.

e: Plateau-Rayleigh instability of ridges within KMC and thin film models Furthermore, results obtained with KMC simulations and continuum thin-film model for the dynamics of the Plateau-Rayleigh instability of ridges formed on a substrate with chemical stripe-like prepatterning were qualitatively compared [Tew17]. It was demonstrated that although the continuum thin-film model results from a long-wave approximation of the Stokes equation, it provides a qualitatively good continuum limit description of the KMC simulations. In particular, we have shown that ridge structures formed in the KMC simulations are subject to a Plateau-Rayleigh instability with well defined time and length scales, well-separated from the intrinsic scales of thermodynamic fluctuations. In Fig. 8 (b, d), the transversal instabilities and the resulting bulges

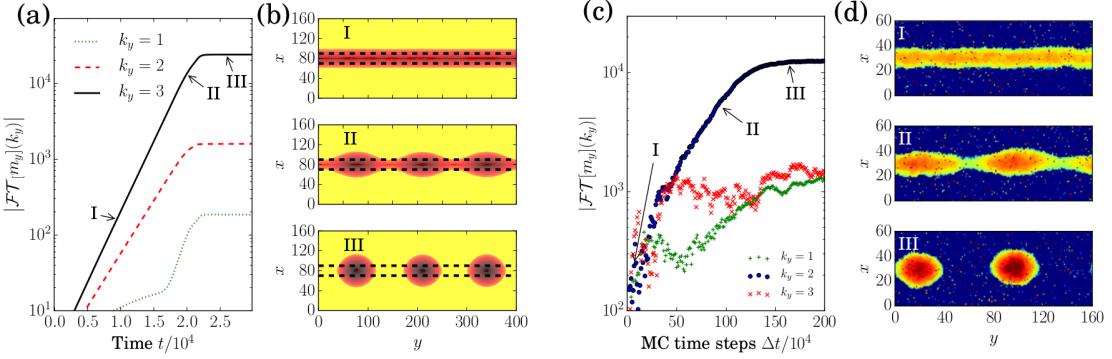


Figure 8: Log-normal plot of the first three Fourier modes over time for the evolution of the transversal instability of the single ridge in (a) a time simulation of the thin-film model and (c) simulation of the LGM model. Snapshots, corresponding to labels I, II and III are shown in (b), (d). The dashed lines in (b) visualize the borders of the more wettable region [Tew17].

on top of the prepattern are shown for both models. In addition, in Fig. 8 (a, c) the time-evolution of the amplitudes of the first three harmonic modes of the transversally integrated field are presented for both approaches. For the continuum thin-film model, the transversal instability develops through an extended phase of exponential growth that corresponds to the linear instability regime. Although in the non-deterministic KMC simulations this regime is influenced by noise, an exponential growth of the mode can still be clearly identified. After the initial linear regime, both models show a nonlinear phase in which the ridge decays into separated droplets via pinch-off events. Although the system is clearly in the nonlinear regime in the later stages of this pinch-off, the growth remains surprisingly exponential, still approximately with the predicted linear growth rate. The extended exponential regime has allowed us to extract dispersion relations from the KMC model via a fitting and averaging procedure [Tew17]. In addition, a system with two neighboring more-wettable stripes was investigated, addressing the question how the weak interaction of two liquid ridges on the two stripes influences their instability (see Fig. 9).

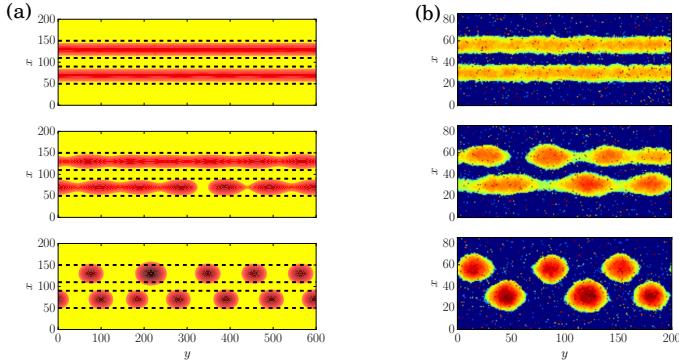


Figure 9: Snapshots from numerical simulations of the transversal instability of two weakly interacting ridges on prepatter stripes. (a) shows results for the thin-film model, whereas in (b) the corresponding results for the KMC simulations are shown [Tew17].

A comparison with dispersion relations, obtained via standard linear stability analysis within the thin film model, has shown a good *qualitative agreement* of the two approaches.

f: Nudged elastic band calculation of the wetting potential The reduction of a stochastic LGM model to a deterministic effective interface model requires two important steps. First, the stochastic model has to be mapped to a deterministic model for the average density field. In [Bul17], a novel numerical Nudged Elastic Band (NEB) approach for the dynamical coarse graining of density dependent energy functional which encode static solutions of the density field and demonstrate it on a simple DFT relevant for the mean field description of the KMC model was introduced. In particular, it was shown that the method yields results that are indistinguishable from those using the fictitious potential method of [28, 37], which

is an approach based on a self-consistent calculation of the fluid density profiles for specified values of the adsorption. Binding potentials obtained with the fictitious potential method were used in [37] to calculate drop profiles that agree remarkably well with drop profiles calculated directly using DFT (see Fig. 10).

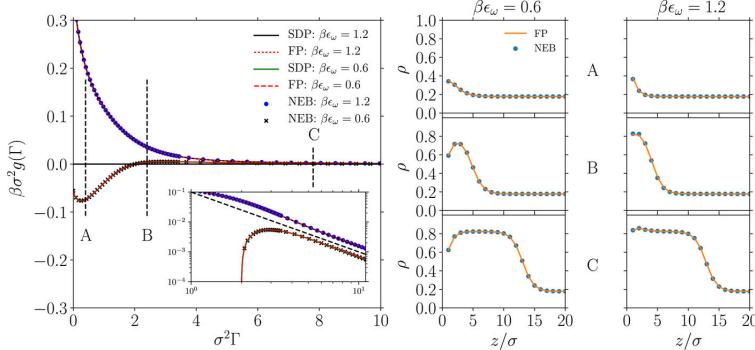


Figure 10: (Left): Comparison of the binding potentials obtained as a function of the adsorption, as determined by three different methods: fictitious potential method (FP), Nudged Elastic Band (NEB) method, and via a pseudo-dynamics that follows the steepest descent path (SDP) in the energy landscape. The inset displays the data in a double logarithmic plot to highlight the power law behavior at large film heights. (Right): The corresponding density profiles are shown for different adsorptions, which are marked in the left panel by vertical dashed lines and the letters A, B, and C, respectively.

The agreement of fictitious potential and NEB approaches represents an important independent validation of the previous results obtained via the fictitious potential approach which have already recently been employed in mesoscopic gradient dynamics models to compute the spreading dynamics of droplets.

g: Others Finally, we would like to mention that the Heuer group has a large expertise in atomistic molecular dynamics simulations which will be required for this project. As a specific example we would like to mention the optimization of polymer electrolytes by including shuttle molecules [Did17]. Furthermore, we would like to refer to the previous development of concepts to describe non-equilibrium behavior in different physical fields from a theoretical perspective (anomalous non-equilibrium behavior upon vapor deposition [Jan15], nonlinear driving, nonlinear conductivity). Also this background is very helpful for the SPP project.

1.3 List of project-related publications

- [Lie12] F. Lied, T. Mues, W.C. Wang, L. Chi, **A. Heuer**, Different growth regimes on pre-structured surfaces: Consistent evidence from simulations and experiments, *J. Chem. Phys.*, 136, 024704, (2012)
- [Jan15] P.K. Jana, W. C. Wang, R.L. Jack, L.F. Chi, **A. Heuer**, Anomalous approach to thermodynamic equilibrium: structure formation of molecules after vapor deposition, *Phys. Rev. E* 92 (2015) 052402
- [Hon15] C. Honisch, T.-S. Lin, **A. Heuer**, U. Thiele, **S.V. Gurevich**, Instabilities of layers of deposited molecules on chemically stripe patterned substrates: Ridges versus Drops, *Langmuir*, 31, 10618, (2015)
- [Wil15] M. Wilczek, W. Tewes, **S.V. Gurevich**, M. Köpf, L. Chi, and U. Thiele, Modelling Pattern Formation in Dip-Coating Experiments, *Math. Model. Nat. Phenom.* 10 (2015) 44-60
- [Wan16] H. Wang, O. Buller, W.C. Wang, **A. Heuer**, D.Q. Zhang, H. Fuchs, L.F. Chi, Area confined position control of molecular aggregates, *New J. Phys.* 18 (2016) 053006
- [Did17] D. Diddens, E. Paillard, **A. Heuer**, Improving the Lithium Ion Transport in Polymer Electrolytes by Functionalized Ionic Liquid Additives: Simulations and Modeling, *J. Electrochem. Soc.* 164 (2017) E3225-E3231

[Tew17] W. Tewes, O. Buller, **A. Heuer**, U. Thiele, **S. V. Gurevich**, Comparing Kinetic Monte Carlo and thin-film modeling of transversal instabilities of ridges on patterned substrates, *J. Chem. Phys.* 146, 094704 (2017)

[Bul17] O. Buller, W. Tewes, A. J. Archer, **A. Heuer**, U. Thiele, **S.V. Gurevich**, Nudged elastic band calculation of the binding potential for liquids at interfaces, *J. Chem. Phys.* 147, 024701 (2017)

[Bul18] O. Buller, H. Wang, W. Wang, L. Chi, **A. Heuer**, Boundary-induced nucleation control: A theoretical perspective, *Phys. Chem. Chem. Phys.*, 20, 3752-3760, (2018)

[Eng19] S. Engelnkemper, **S. V. Gurevich**, H. Uecker, D. Wetzel, U. Thiele, Continuation for Thin Film Hydrodynamics and Related Scalar Problems, in *Computational Modelling of Bifurcations and Instabilities in Fluid Dynamics*, ed. A. Gelfgat, p. 459–501, (2019)

2 Objectives and work program

2.1 Anticipated total duration of the project

36 Months

2.2 Objectives

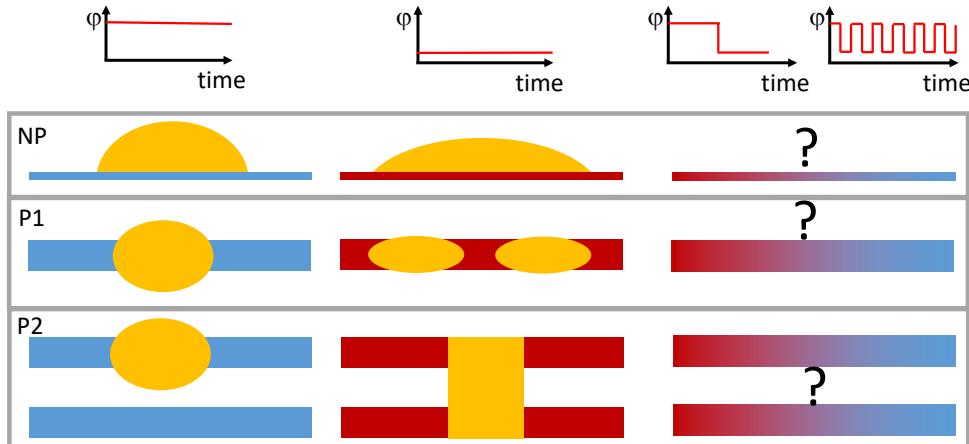


Figure 11: Sketch of the different geometries analyzed in this project. Case NP (no prestructure): Droplet on a switchable homogeneous substrate. Case P1: Droplet at one- and Case P2: Droplet at two close-by stripes, formed from SAMs of switchable molecules. The key questions deal with the effect of a time-depending switching protocol, yielding a complex non-equilibrium response.

The key goal of our theoretical project is to study the impact of *switchable prestructured substrates* on the resulting wetting behavior of simple liquids. Here we start with a general classification of our project with respect to the systems as well as physical properties to be analyzed, the different numerical/theoretical approaches, and the multiscale techniques to bridge between them on a quantitative level. More details will be found in the subsequent WPs.

Systems and physical properties: We aim to describe the wetting behavior of simple liquids for switchable substrates. The general questions are sketched in Fig.11. On the one hand, we consider a homogeneous

substrate (case NP) where the properties of the droplet (e.g., contact angle) change as a function of the interaction between substrate and droplet. On the other hand, we study the switching between the two different states, occurring for one stripe (P1) or for pairs of stripes (P2). In both cases the non-equilibrium properties will be studied which emerge upon switching of the photoactive molecules. In general, one may expect significant variations of the topology of the non-equilibrium structures as compared to the original configurations. A particularly interesting non-equilibrium situation can be generated if the switching occurs periodically so that a stable non-equilibrium state is generated for long times with properties depending on the switching frequency.

For the different cases there exist several experimental projects in the SPP for a closer comparison, based, e.g., on photoactive molecules (**B. Braunschweig** and **B.J. Ravoo**), shape-changing polymers (**L. Ionov**), freely-rotating Janus particles (**A. Syntska**), laser-nanostructured micro-channels (**O. Varlamova/R. Borcia**), membranes (**T. Pfohl/U. Steiner**), or smectic liquid crystals (**R. Stannarius/A. Eremin**). Via the direct interaction with experimental groups we aim to advance the control of collective transport of molecules on prestructured switchable surfaces and overall quality control and error suppression. The expected results will help to optimize the preparation conditions to obtain complex self-assembly structures over large experimental parameter ranges.

Different numerical/theoretical approaches: In general, the molecular structure of an interfacial layer and its interactions with the liquid phase determine the switching kinetics at the interface. Furthermore, the latter changes at the molecular scale of the interface, driving the behavior on micro- and macro-length scales like the wetting properties of the solid surface. For that reason, we believe that structure-property relations from the interfacial to the mesoscopic level exist and can be used to control wetting of a switchable substrate reversibly. On the molecule/particle level the dynamical behavior will be modeled by MD, MC simulations of a LGM and DDFT approaches. On the mesoscopic continuum level we use thin-film models, using a gradient dynamics on interface Hamiltonians. The continuum equations help to analyze possible instabilities of the liquid structures.

Multiscale techniques: Given the advantages and disadvantages of the different theoretical and numerical methods, it is evident that a mapping between the methods is of great interest. To this aim, a bridging microscopic Density Functional Theory will be employed in the parameter passing between the microscopic stochastic LGM level and the mesoscopic deterministic continuum level. Furthermore, a direct bridge between the atomistic MD level and the mesoscopic level will be used. The developed matched hierarchy of models shall allow us to quantitatively understand crucial aspects of non-equilibrium effects across several length and time scales. The results gained with the developed multiscale theory will be compared and exchanged with several theoretical groups in the SPP: thin-film gradient dynamics models for adaptive substrates (**U. Thiele**), boundary element method for solving the Stokes equation for the droplets dynamics at substrates with switchable wettability (**H. Stark**) or phase-field models (**O. Varlamova/R. Borcia**). Furthermore, we will compare our results on parameter passing with alternative approaches, governed by MD simulations (**T. Speck/P. Virnau**). The parameter passing method will be also applied to other projects in the SPP, e.g., for matching of mesoscopic models for simple liquid on adaptive brush (**U. Thiele**).

2.3 Work program including proposed research methods

The project is organized into 3 work packages, labelled WP 1-WP 3 in the following.

WP 1. Structure formation on switchable substrates: A microscopic perspective (Heuer) One primary goal is to study the time-evolution of the resulting structure formation after the switching process as well as the non-equilibrium steady state in case of fast switching. Although the conceptual multiscale aspects of this project are independent of a specific experimental realization, we will explicitly refer to experimentally studied systems in this SPP.

WP 1.1. Molecular dynamics simulations of a water droplet on a self-assembled monolayer In the projects by **B. Braunschweig** and **B.J. Ravoo** via contact printing of self-assembled monolayers of the photoactive molecule arylazopyrazole on appropriate substrates, homogeneous surfaces as well as stripes with nanometer to micrometer periodicities will be generated. Upon irradiation of light the molecules change their conformation which goes along with a change of the surface properties [46] and thus change the wetting behavior of water. Due to the large number of accessible physical chemical properties in the planned experimental studies of the Braunschweig group (e.g. molecular structures, charging state of interface, dynamic surface tension, contact angles, pressure-height correlations) a close comparison with our theoretical project is envisaged.

We will study the properties of that system via MD simulations. Of relevance are the different interfacial tensions, characterizing the system. Atomistic simulations of the wetting of water on photo-switchable azobenzene moieties is indeed feasible [25]. The MD simulations will be performed using GROMACS together with the general Amber force field [47]. Individual simulations of the cis- and trans-conformation of arylazopyrazole will be performed. Standard ways to determine the interfacial tension is either on basis of the difference between the normal and the tangential pressure across the boundary region or by using the Kirkwood-Buff formula [48] Whereas the original approach is applicable for pair-wise potentials, the application to multi-body terms, required for realistic microscopic simulations, is relatively complex. Therefore, we also plan to use the more general test area method, based on reweighting techniques which does not require the calculation of the pressure contributions and is thus independent of the chosen force field [49, 50]. In particular, this information will serve as an input for WP 1.2 and WP 1.3.

In a second step we will simulate a water droplet on the homogeneously covered substrate, using both the trans- and cis-conformation and compare the resulting contact angles with the expectation based on the interface tensions [51]. Care must be taken with respect to the finite size of the droplet [52].

Whereas these two steps are standard but essential as a sound basis for this project, a new aspect refers to the non-equilibrium dynamics of the droplet after switching the photoactive molecule, corresponding to case NP in Fig.11. Technically, the switching can be realized in different ways. First, one uses the droplet shape of, e.g., the trans-conformation and initializes the water molecules with this shape on the substrate with the cis-conformation. This allows one to observe the subsequent non-equilibrium approach of the water droplet to the new equilibrium state. Although the complete equilibration process may be out of reach for these detailed MD simulations, already the initial equilibration may be of help for comparison with simulations in WP 1.2 or WP 1.3, using simpler models. A new aspect would enter, if one uses the time evolution of the switching process. For this purpose a reactive rotation potential and switching functions have been developed based on QM calculations [53, 54]. This would allow one to reproduce the collective switching process upon isomerization. This approach is readily implemented in GROMACS. Whether or not this approach is already performed here or shifted to the years 4-6 of this project, depends on the progress in the remaining part of this workpackage.

WP 1.2. Exploration of non-equilibrium effects via Molecular Dynamics simulations of a model system As discussed above, for simple force fields (e.g. Lennard-Jones-type) it is possible to obtain detailed atomistic information about the wetting behavior. Naturally, this requires a sufficiently large number of particles ($10^5 - 10^6$). Similarly to the LGM, three energy scales (relative to temperature) are important. The energy scale ϵ_{pp} of the interaction between the particles, representing the water, sets the scale for the liquid-gas transition. The interaction of the particles with a substrate is characterized by ϵ_{ps} and can be obtained by reproducing the contact angle for a droplet on that substrate. Based on this model, case NP of Fig.11 will be simulated for the different switching scenarios to analyze the specific non-equilibrium effects. Several goals can be formulated. First, the parameters are adjusted to agree with the macroscopic input from the experimentally oriented projects so that a direct comparison becomes possible. Second, for the specific case of the switching of photoactive molecules it will be checked in comparison with WP 1.1, to which degree the use of a simplified model in this WP changes the observed equilibration process upon switching between both isomers. Third, simulations of particularly interesting scenarios are performed such as fast transitions

between a strong hydrophilic case (contact angle much smaller 90°) and a strong hydrophobic case. Fourth, one may analyse in detail for the case of fast switching the impact on the individual particles. One may guess that the reaction of the particles on the switching depends on the distance. Thus, a detailed analysis with respect to the fluctuations of the height of the droplet at the different locations of the substrate may yield important insight which may be relevant, e.g., for the understanding of the non-equilibrium behavior and for the interpretation of the thin film approach.

WP 1.3. Exploration of non-equilibrium effects via Monte Carlo simulations of a Lattice Gas Model

Similarly to the continuous model system from WP 1.2 the LGM is based on three energy parameters which will be determined in the same spirit as in WP 1.2 (relative to temperature). We will use the interaction scheme from Ref. [28] in order to reduce effects of the underlying lattice on the resulting structures. In order to be able to analyze also cases P1 and P2 from Fig.11, the energy scale ϵ_{ps} has to be determined for the different cases of interest (here: with photoactive molecules (trans and cis-isomers) and without photoactive molecules). In order to keep the information about relative time scales, the attempted swaps are restricted to nearest neighbor positions [55].

Due to the increased efficiency in contrast to MD simulations, we aim to simulate all three scenarios from Fig.11 via Monte Carlo simulations. Again, in the same spirit as WP 1.2 we will consider all experimentally relevant cases in this SPP. For case NP it will be interesting to see, how the relaxation starts after switching the interaction between the particles and the substrate. Among others it will be checked whether the resulting droplet shape in case of fast switching between both types of substrate reflects the equilibrium case of an intermediate interaction value. The results will be compared with the MD simulations (in their accessible time regime) in order to estimate the impact of the inherent coarse graining procedure for the present application.

Going beyond the preliminary work for case P2 from Fig.11, as outlined above, we first extract the range of geometric parameters (width and distance of stripes, number of particles) for which both the bulge and bridge configuration are equally likely in terms of their free energies. Preliminary work indicates that in case of large droplets and the corresponding larger time scales Umbrella Sampling [56] is even more efficient than Markov State Modelling for this analysis. Then, small variations of the interaction parameters may give rise to the desired switching process between the bulge and the bridge configuration. For these geometries we then analyze in detail the two switching protocols, shown in Fig.11, and characterize the resulting non-equilibrium behavior. Large spatial rearrangements are expected, which may give rise to interesting non-equilibrium structures.

WP 2. From a microscopic to the mesoscopic effective interface description (Heuer/Gurevich)

WP 2.1. Statics A key aspect is the quantitative connection of the coupled deposition and non-equilibrium rearrangement dynamics of molecules on pre-structured substrates on the microscopic level with mesoscopic continuum models, namely, gradient dynamics based on an effective interface description. One example are hydrodynamic thin-film models as used individually in [Hon15, Wil15]. This will be individually performed for the MD simulations from WP 1.2 and the MC simulations from WP 1.3. The quantitative connection shall be achieved via appropriate *parameter passing methods*. In a first step this involves the mapping of the equilibrium behavior, i.e., their statics/energetics. The developed parameter passing methods for interface tension and the effective wetting potential shall then be applied to different homogeneous substrates to then generalize the results to the heterogeneous substrates. The resulting interface Hamiltonian (or free energy) is then incorporated into the mesoscopic continuum model (cf. WP3) to show that height profiles of mean field droplets obtained from microscopic approaches are accurately reproduced for homogeneous and heterogeneous substrates.

For the MD simulations we follow the parameter passing procedure from [39]. In this way we extract the different tensions as well as the effective wetting potential/disjoining pressure, exploring different types of

virial information. For pair-potentials this approach is straightforward, albeit technically demanding. This approach may be compared with the mapping procedure in the project of (**T. Speck/P. Virnau**).

A detailed comparison of simulations of the discrete LGM and a continuous thin-film model have revealed strong similarities [Tew17]. These results suggest that also a LGM can be successfully mapped on a continuous level. Here we will apply an approach based on a fictitious potential as developed for lattice DFT in [28, 37] and an efficient nudged-elastic-band approach to parameter passing [Bul17]. For this purpose we will perform a lattice DFT analysis based on the parameters of the LGM. Indeed, height profiles of mean field droplets obtained from the lattice DFT are accurately reproduced for homogeneous and heterogeneous substrates.

WP 2.2. Dynamics The mapping on a purely energetic level does not only allow one to investigate static ridge and droplet states but also to assess their stability either via a second variation of the free energy or via a dynamical approach. Second, the parameter passing methods will be extended towards the dynamic behavior, i.e., kinetic (non-equilibrium) characteristics as transport coefficients (diffusion constants, slip length, effective viscosities) will be extracted from MD, MC and DDFT simulations. In parallel, the mesoscopic model in gradient dynamics form is extended to capture different transport channels (see WP 3.1), i.e., a combined Cahn-Hilliard and thin-film type is used [57]. Their relative weight is also extracted from the microscopic level.

Our approach is general and results can be used for other projects within the SPP: For example, one can obtain wetting and surface energies via parameter passing matching micro and mesoscopic models for a drop of a simple liquid on an adaptive brush (**U. Thiele**).

WP 3. Calculations on the mesoscopic level (Gurevich)

WP 3.1. Thin film model extension On the level of mesoscopic continuum models, we have already successfully applied a thin-film model to explain the transport mechanisms and structure formation during the redistribution stage of deposition experiments [Hon15, Tew17]. Thereby, the periodic prepattern is introduced as a chemical heterogeneity that affects the wettability and is incorporated as a spatially modulated wetting potential. In order to introduce a (periodic) switchable dynamics, this spatially modulated wetting potential will be additionally modulated (periodically) in time. This hydrodynamic thin-film model shall be then extended to capture both, transport by diffusion at very small (sub-monolayer) film height and by advection at larger film height, including the transition between the two transport channels. This will be achieved by the introduction of more complex mobility functions. A discussion of these transport modes in the context of a thin film evolution equation with a general polynomial mobility function can be found in [58]. Thereby, the relative weight of the different transport channels is also extracted from the microscopic level (see WP 2). As our thin film approach is general and can be applied to many related systems. It also allows for the incorporation of certain lateral driving forces. Hence we envision an exchange with other projects using mesoscopic models liquid dynamics. This includes the projects on thin-film gradient dynamics models for adaptive substrates (**U. Thiele**) or phase-field models (**O. Varlamova/R. Borcia**). We will also collaborate with the project of (**H. Stark**), who also works on droplet dynamics at substrates with switchable wettability using a boundary element method for solving the Stokes equation. We will identify special test cases in order to compare our results.

WP 3.2. Direct numerical simulations The developed efficient numerical routines based on finite difference and finite element methods already allow for large-scale two-dimensional direct numerical simulations [45]. These routines can now be readily adapted for any such model developed in the project. A preliminary numerical simulation example is presented in Fig. 12 that shows three snapshots from a time simulation of the thin-film model for nine weakly interacting liquid ridges on a pre-structured substrate for standard hydrodynamic mobilities. Here, one can see that the bulges are formed subsequently due to

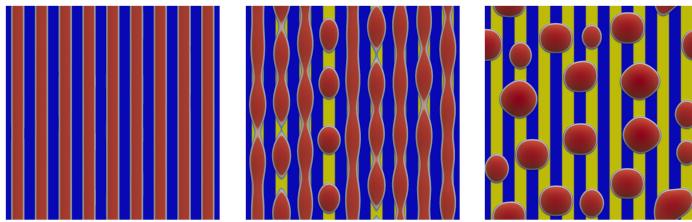


Figure 12: Three snapshots of a 2D numerical simulation of the thin-film equation with nine prepatterned stripes. One can see how bridge structures between adjacent stripes form due to coarsening of the bulges.

transversal instability of the ridges and the bridge structures emerge due to coarsening of the bulges. We aim to incorporate the effect of a (periodic) switching and systematically investigate different geometries starting with the cases of droplets on homogeneous switchable substrate and of one and two switchable stripes (cf. Fig. 11, cases NP, P1, P2, respectively).

For the static homogeneous substrate, the change in the wettability results in the different static contact angle (cf. Fig. 11). If the periodic switching is introduced, the system reaction will depend on the ratio between the time scale given by switching and the reaction time of the liquid. We are going to systematically investigate these changing of the contact angle during the switching, especially concentrated on the case of fast switching.

In the case of one switchable stripe, the change in the wettability results may result in either migrating of the droplet from more- to less-wettable stripe by switching or by the droplet may split in two if enough volume is presented. Both situations may lead to a complex dynamics by periodic switching, again, we will specially focus on the case of fast switching.

In general, on a static homogeneous substrate, no stationary two droplet configuration can be found where the distance of the droplets is not equal to the half of the domain size. However, for the prepatterened substrate such solution can be obtained [Tew17]. There, two transversal eigenmodes become unstable: The first mode proceeds through periodic transversal mass transfer equally in both ridges, whereas the second mode also includes mass transfer between the two ridges such that a relative shift by half a period results, indicating the weak interaction of the ridges. One question that will be addressed is how this morphology will change by switching? What kind of new stable droplet configurations will form by changing the distance between prestructures, a contrast of the prestructure and the switching frequency. Another interesting question is how the weak interaction of two liquid ridges on the two stripes influences the stability properties and how different mobilities influence the balance between the different instability modes.

Finally, the effect of coarsening by switching will be discussed in details. The coarsening of droplets and ridges on the homogeneous substrate occurs due to two main mechanisms: mass transfer through the adsorption layer and coarsening through coalescence of neighboring drops. While the latter mechanism can be suppressed by introducing prestructure, which results in pinning forces, the coarsening through diffusion can play an important role for the stability of liquid structures on static prepatterened substrates. We are aiming to investigate the effect of the mass diffusion for different distances between the prestrucures and the switching parameters. For all of the planned issues we will give our expanded numerical algorithms into a pool of tools available to all projects within of SPP.

For all cases we will compare the results obtained by a numerical simulations with results form experimental projects in the SPP. One of the particular system deals the time-depending switching dynamics of structured substrates based on freely rotating Janus particles (JP) with the resulted non-equilibrium wetting behavior of water (**A. Syntska**). We expect that JPs will build up structured surfaces with different complex geometries (hexagonal or stripes), patchiness, and wettability (less or more wettable) depending on the topologies (spherical or rod-like) as well as hydrophobic/hydrophilic contrast. The key questions are what happens (i) with the dynamics of water droplet during the switching process; (ii) with dynamics of the droplet if formed surface from JPs will be chemically homogeneous; (iii) with dynamics of droplet if formed surface from JPs will be chemically prestructured; (iv) with the dynamics of droplet if formed surface from JPs will be topographically prestructured. Other experimental systems involve photoactive molecules

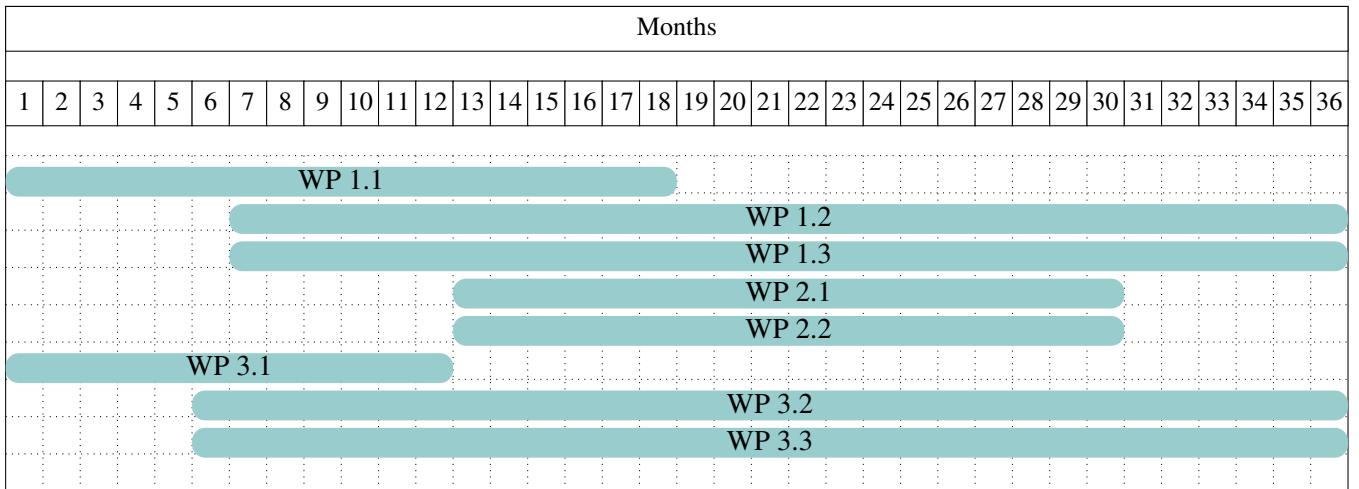


Figure 13: Time line and data flow in the project.

(**B. Braunschweig**) and (**B.J. Ravoo**), shape-changing polymers (**L. Ionov**), laser-nanostructured micro-channels (**O. Varlamova/R. Borcia**), membranes (**T. Pfohl/U. Steiner**), or smectic liquid crystals (**R. Stan-narius/A. Eremin**).

WP 3.3. Path continuation The unstable states represent important transients that structure the time evolution where they result in prominent plateaus in the free energy [Hon15]. Hence we expect that these unstable steady states are the ones that are most easily stabilized through imposed spatio-temporal patterning. As unstable states cannot be reached by direct numerics, the time simulations shall be supplemented by *path following methods* that can efficiently track the entire solution structure and its stability.

Efficient two-dimensional continuation tools were developed recently and successfully applied to thin film equation. However, the bifurcation analysis of the system involving explicit time-dependence, in our case the switchable dynamics, is very tedious: The standard continuation procedure is based on the tracking stationary, time-independent solutions. However, several steps will be performed in order to include the switchable dynamics into the continuation: (i) We start with a continuation of steady state solution of the thin-film equation corresponding to different constant wettabilities. The stable and unstable solutions will be analyzed in detail and compared with each other. This will give us a hint about possible transition behavior; (ii) In case, where the switching frequency is small, the time-dependent term can be expanded and corresponding linear stationary problem will be analyzed and compared with the full system by means of time simulations (cf. WP 3.2); (iii) Finally, in case of periodic switching, time-periodic dynamics will emerge. The latter can be seen as a *time periodic orbit*, emerging from a stationary solution when we increase switching parameters from zero. This situation can be analyzed within already developed tools (see e.g., [44,45], [Eng19]). With the aid of these advanced numerical tools, we will also able to investigate complex switchable prepatterned geometries in detail, starting again with the case of homogeneous switchable substrate. On each step, the hand-on tutorials explaining the technical continuation details will be prepared and made online freely available.

Time line of the project. Figure 13 represents the time line of the project.

2.4 Data handling

The research data gained from the project will be handled according to the guidelines of the Westfälische Wilhelms-Universität Münster (WWU). All scientific results will be published in international peer-reviewed journals and be presented at conferences. Following our past practice, all manuscripts will also be uploaded

to the preprint server arXiv so that full open access is guaranteed. Furthermore, we plan to bring essential parts of the developed continuation and time stepping algorithms into tutorial form and make them available to the wider community.

2.5 Other information

Not applicable.

2.6 Explanations on the proposed investigations

No experiments on humans, human materials and animals are planned.

2.7 Information on scientific and financial involvement of international cooperation partners

No close collaboration with researchers based outside Germany is planned.

2.8 Information on scientific cooperation within SPP 2171

In the framework of SPP we aim to analyze the dynamics of a simple liquid on switchable pre-structured substrates in a close collaboration with both experimental and theoretical projects within the SPP. In particular,

(i) We aim to compare our theoretical predictions with the results from several experimental groups working on dynamics of switchable substrates based on photoactive molecules (**B. Braunschweig** and **(B.J. Ravoo)**, shape-changing polymers (**L. Ionov**), freely-rotating Janus particles (**A. Synytska**), laser-nanostructured micro-channels (**O. Varlamova/R. Borgia**), membranes (**T. Pfohl/U. Steiner**), or smectic liquid crystals (**R. Stannarius/A. Eremin**). The expected results may help to optimize the preparation conditions to obtain complex self-assembly structures over large experimental parameter ranges;

(ii) The results gained with the developed multiscale approach will also be compared with several theoretical groups working on both micro and mesoscale modeling within the SPP: It includes thin-film gradient dynamics models for adaptive substrates (**U. Thiele**), a boundary element methods for solving the Stokes equation for the droplets dynamics at substrates with switchable wettability (**H. Stark**) or phase-field models (**Varlamova/Borgia**).

In addition, to foster the exchange between theoretical groups working with continuum-theoretical approaches within the SPP, we have initiated an informal network, which includes the groups of **S. Gurevich**, **D. Peschka**, **J. Snoeijer**, **H. Stark**, **U. Thiele**, and **B. Wagner** and is open to others. There, we will co-ordinate aspects of the training of the involved young researchers within the SPP, and meet sporadically to discuss details of our approaches and ongoing work.

(iii) We also plan to collaborate with several groups working on parameter passing methods and their applications. We will compare our results on parameter passing from the lattice and the continuum level with approaches, used for MD simulations of complementary systems (**T. Speck/P. Virnau**). In particular, a direct exchange of results and technical issues may give rise to strong synergy effects among the groups. The developed methods are general and can be applied to other projects dealing with multiscale dynamics of liquids (**Thiele**).

3 Bibliography concerning the state of the art, the research objectives, and the work program

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4 Requested modules/funds

4.1 Scientific personnel

3/4 TVL-13 annually	48 375 €
3/4 TVL-13 annually	48 375 €
Sum	290 250 €

Justification The PhD positions will be based on 75% TVL E13, according to 2018 DFG personal cost rates amounting to 64 500 € for the full PhD position per year.

1. Doctoral Student (requested by S. Gurevich, 3/4 TVL-13, 36 Months), who will process the WPs 2 and 3 of the project. The position will include the theoretical and numerical modeling of the thin-film equation, developing of two-dimensional continuation method as well as parameter passing methods. The PhD student should have a strong background in nonlinear physics and numerical treatment of nonlinear partial differential equations.
2. Doctoral Student (requested by A. Heuer, 3/4 TVL-13, 36 Months), who will process the WPs 1 and 2 of the project. The doctoral student will perform the MC and MD simulations and will be also involved in the parameter passing methods as a cooperation between both groups. A strong background in MC and MD simulations is required.

4.2 Travel costs

SPP workshop, 1st+2nd year	5000 €
Advanced School, 1st year	1500 €
Phd Workshop, 2nd year	1500 €
SPP conference, 3rd year	5000 €
Sum 1	13 000 €
Other travel costs (annually)	4 000 €
Sum 2	12 000 €
Sum 1+2	25 000 €

Justification

- Travel money are planned allowing PIs and the employed PhD students to attend SPP events;
- Other travel expenses are planned for the PhD students and the PIs. The travel funds will be used to present the research results to an international audience at conference meetings.

4.3 Publication costs

Publication cost annually	750 €
Sum	2 250 €

5 Project requirements

5.1 Employment status information

- PD. Dr. Svetlana Gurevich: Research assistant (Akademische Rätin a.Z.), fixed-term contract till 01.07.2019; A position commitment till 01.10.2022.
- Prof. Dr. Andreas Heuer: Full Professor, permanent position.

5.2 First-time proposal data

No

5.3 Composition of the project group

1. Prof. Dr. Andreas Heuer is responsible for guiding the doctoral student, for the interaction with other experimental and theoretical groups, and for publishing the results (paid by the university).
2. PD Dr. Svetlana Gurevich is responsible for guiding the doctoral student, for the interaction with other experimental and theoretical groups, and for publishing the results (paid by the university).
3. PD Dr. Volker Weiss is guiding the MD simulations of the doctorate student and performing some simulations by himself (paid by the university).

5.4 Cooperation with other researchers

5.4.1 Researchers with whom you have agreed to cooperate on this project

See Sec. 2.8 for details

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

- Prof. A. J. Archer, Loughborough University, UK
- Prof. U. Thiele, WWU Münster, Germany
- Prof. H. Fuchs, WWU Münster, Germany
- Prof. L. Chi, Suzhou University, China
- Prof. T.-S. Lin, National Chiao Tung University, Taiwan
- Prof. Mustapha Tlidi, Universit libre de Bruxelles, Belgium
- Prof. Julien Javaloyes, Universitat de les Illes Balears, Spain
- Prof. Oliver Pierre-Lois, University of Lyon 1, France
- Prof. R.L. Jack, Cambridge, England
- Prof. D. Bedrov, Utah
- Prof. O. Borodin, Washington
- Prof. C. Holm, Stuttgart
- Prof. S. Egelhaaf, Düsseldorf

5.5 Scientific equipment available for the project

1. HPC cluster Palma II of the WWU Münster (among the TOP 500 in 2018)
2. HPC cluster of AK Heuer (approx. 100 nodes)

5.6 Project-relevant interests in commercial enterprises

There are no connections between the project and the production branch of the enterprise.

6 Additional information

This proposal has not been submitted to a third party.