**Project Description – Project Proposals**

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***Dynamic De-wetting: Droplets on Sonically Switched Surfaces ($D^3S^3$)***

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**Project Description**

## 1 State of the art and preliminary work

*State of the art*

The understanding of the dynamic behaviour of a droplet on a vibrating substrate is of fundamental and technological importance in many scenarios, like evaporation [Mor17] or droplet atomization [Jam03]. Experiments regarding vibrating droplets have therefore received much attention in the past. Some examples from the literature are given in the following without claiming completeness. In [Smi89] the authors experimentally determine the resonance frequencies of microscopic mercury droplets and identify different types of vibrations. The spreading of a droplet on vibrating non-wetting surfaces is investigated in [And94]. The authors find a simple relation for the contact angle after vibration and the contact angle hysteresis. Experiments on vibrating droplets have also led to advances in contact angle measuring methods. In [Mei04] measurements of the diameter and weight of a droplet on a vibrating real (rough) surface are used to determine the contact angle. The results agree with the Wenzel equation. A controlled vibration of the substrate can also be used to define the motion of a droplet on a substrate [Dan05], which makes it possible to control droplet transport, mixing, and thermal cycling. The scale-bridging between vibrating droplets of different sizes is not trivial. In [Cel06] the authors find that their scaling law for the energy dissipation within a droplet is not valid across scales. For small droplets they detect a contact line movement for weak substrate accelerations for which a fixed contact line would be expected when taking the behaviour of larger droplets as a basis. In [Moo06] it is found that the lowest oscillation mode of a pendant drop is not, as thought before, the longitudinal vibration but the rotation of a drop around the longitudinal axis. A vertical vibration of the substrate can be used to control the wetting state of a droplet. The authors of [Lei14] investigate the Wenzel to Cassie state transition and find that the vibration amplitude that is needed for the transition at a given frequency decreases when the distance between the pillars of their microstructured surface increases.

Vibrating droplets have not only been investigated experimentally but also by continuum models. In [Bas94] a finite element model is used to compute the nonlinear oscillations of pendant droplets. Their results show that an increase in the initial droplet deformation can lead to an increase or decrease of the oscillation frequency depending on the size of the droplet. This emphasizes once more the complexity of the scale-bridging for different droplet sizes. Continuum models can also reveal the resonance frequencies of sessile droplets [Wil97]. The simulations of [Don06] give an estimation of the contact angle variation of droplets sitting on a laterally vibrating substrate.

While much work has been done regarding droplets on vibrating substrates in general, droplet detachment due to vibrations has only received little attention. In [Kim04] the authors experimentally find resonance frequencies at which a droplet falls from a vibrating ceiling. The detachment of droplets from a vibrating membrane can be used to produce uniform and very small emulsions [Zhu05]. The experimental results of [Shi14] indicate that a complete detachment of small-scale droplets happens only at the second mode. Using the volume-of-fluid method droplet ejection from a vertically vibrating surface is investigated by a continuum model in [Jam03]. Applying molecular dynamics simulations, the authors of [Niu14] evaluate the dynamic behaviour of droplets on smooth and rough vibrating surfaces. Besides the aforementioned Wenzel to Cassie state transition they also observe a detachment of the droplet when enhancing the vibration.

Hence, despite its importance, only little is known up to now on the rich phenomenology of the detachment of droplets from vibrating surfaces. The present project aims at contributing to our understanding of the interesting and complex process by an approach in which atomistic simulations are consistently combined with phase field simulations and experimental studies.

*Preliminary work*

The applicants have collaborated previously in studies of wetting of surfaces within the Collaborative Research Centre 926 (CRC 926) “Microscale Morphology of Component Surfaces” (MICOS). In this collaboration a unique approach was developed, in which atomistic simulations (carried out by molecular dynamics) and continuous simulations (phase field method) are consistently combined. Atomistic simulations enable the investigation of wetting on the nanoscale, while phase field simulations enable a coupling to larger scales, especially the microscale. Additionally, wetting was also investigated experimentally.

For the molecular dynamics simulations, the efficiently scaling code *ls1 mardyn* [Nie14] was used, which presently holds the world record in system size in molecular dynamics simulations [Eck13]. Classical molecular dynamics simulations rely on force fields that describe the interactions of particles. For a given force field, simulation results are predictive, i.e. no further parameters are introduced. Because of this predictive nature of molecular dynamics simulations, not only single properties, but also the coupling of different phenomena can be investigated (e.g. adsorption and wetting) [Hor13a,b, Hor14, Hor15, Wer13, Wer15a,b,c, Wer16a,b, Wer17a,b]. In CRC 926 the wetting of surfaces was investigated systematically for systems with dispersive interactions [Bec14, Bec17]. In a related study, that was completed very recently (the manuscript is under review) the adsorption in the same systems was investigated, so that now consistent quantitative data on both adsorption and wetting in these systems is available. In addition, in the same study, the influence of interactions on the thickness and structure of the adsorption layer and the transition to droplet formation was investigated. Also metastable states of the fluid were considered. Not only planar surfaces [Bec14] but also structured surfaces were considered [Bec17]. In the latter also dynamic wetting processes were investigated. These studies give a consistent picture of wetting and adsorption. They also give fully detailed atomistic information on the zone where all the three phase are in contact (contact “line”).

In the applicants’ preliminary work in CRC 926 a scale-bridging method was developed that enables transferring the results from atomistic simulations to larger length and time scales. To this end, methods and tools were developed for the description of wetting processes using phase field models. These continuous methods are based directly on our atomistic simulations.

A decisive component of phase field models is the free energy density function. This function determines the properties of interfaces and bulk phases. In many works concerning phase field modelling, this function is chosen ad hoc. Hence, no physical conclusions can be drawn concerning thermodynamic properties of the interfaces themselves. By correctly choosing these functions, wetting properties, as e.g. the contact angle can be prescribed [Sai14]. In previous work from our group, the free energy density function is coupled directly to molecular modelling and simulation. Thereby, the results of the phase field simulations become physically meaningful also in the transition layer between two bulk phases.

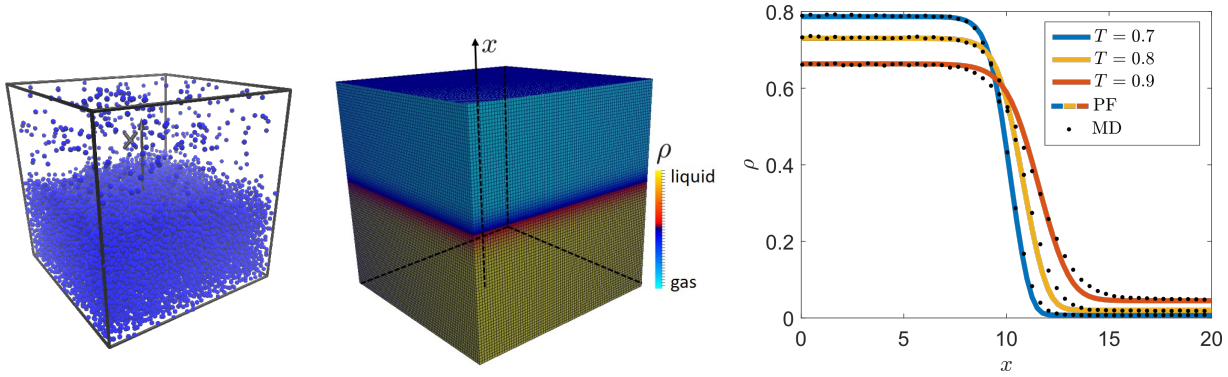



**Figure 1:** Simulation results for nanoscale density profiles at a vapor-liquid interface with different methods. Left: Snapshot from molecular dynamics simulation, middle: Density field from phase field simulation, right: Density profiles for different temperatures *T* (dimensionless property, reduced by LJ units). The density profiles of the phase field simulations show good agreement with those from molecular dynamics simulations [Die18b].

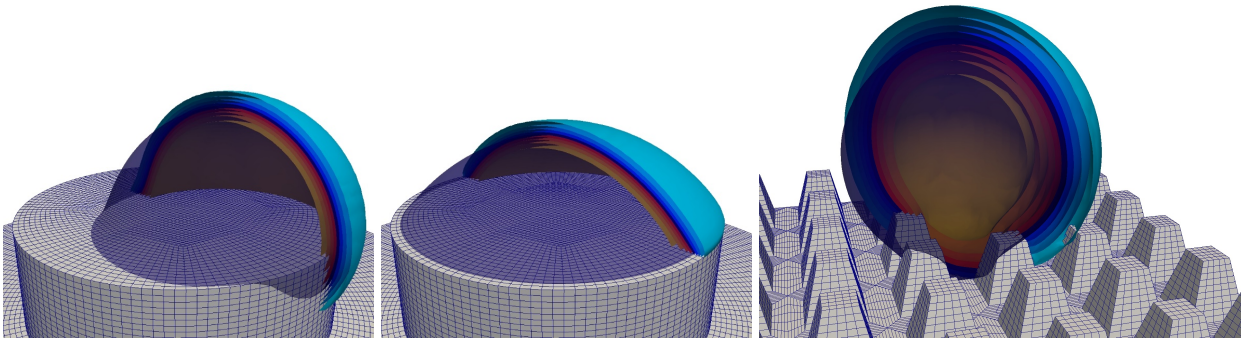
In previous work we used the Lennard-Jones truncated and shifted model with a cut-off radius of $r_c = 2.5\,\sigma$ as model fluid (LJTS fluid). The LJTS fluid is a popular model fluid because of its simplicity and the resulting advantages in simulation techniques. It describes the properties of simple real fluids very well. For this fluid, we have developed an equation of state (PeTS: perturbed truncated and shifted), which very accurately describes its properties in the stable and metastable range [Hei18a]. Because of the favourable properties of the equation, it allows the investigation of interfacial properties with density gradient theory (DGT) or classical density functional theory (DFT), respectively. For the latter, the according functional was developed [Hei18a]. Using DGT or DFT, macroscopic properties like the interfacial tension, but also nanoscale properties like the structuring of fluids in the vicinity of surfaces can be described [Wer16b, Kel17, Ste18]. In the area of DFT, we closely collaborate with the group of Prof. Chapman, Rice University, Houston, Texas, USA. DGT and DFT can be applied to adsorption. Usually DFT and DGT are applied to one-dimensional planar stationary scenarios (see e.g. [Mai17]). The phase field method is an elegant approach for extending this to arbitrary 3D scenarios, including transient situations.

In our approach, the free energy density from PeTS equation of state is used in the phase field model. The results of the phase field model are thereby consistent with those of molecular simulation, see figure 1 and [Die18b]. However, in the phase field model the fluctuations, that are present in molecular simulation, are not represented. Furthermore, there are different options to include the fluid-wall interaction in the phase field model. In the published preliminary work of the authors, this was done by boundary conditions. Surface tensions were assigned to surface elements in such a way that the contact angle of the droplet, which is known from the molecular simulations, was matched. The gas-liquid surface tension in the phase field model is correct by virtue of the constitutive equation, which is based on the PeTS equation of state and the DGT. Hence, in this version neither the nanoscale structuring of the fluid near the wall nor

the adsorption, which are present in the molecular simulations, are described by the phase field model. These effects can be included explicitly in the phase field model by using wall potentials. The corresponding extensions are presently being carried out within CRC 926 and will be available for the work in the present project. However, in the first funding period of the present project, we will focus on the well-established description of the surface elements described above.

The phase field approach as a simulation method is very flexible and allows the investigation of complex scenarios such as the coupling between fluid and solid mechanics. The implementation of PeTS equation of state in the phase field method was supported by the use of hyper-dual numbers [Fik11], which allow automatic differentiation of the expressions the free energy. This approach renders the cumbersome and error-prone exchange of equations of state quick and robust. Thereby, the phase field model can easily be adapted to different fluids, which can be treated more easily in experiments [Die18b]. To the best of our knowledge, this is the first use of hyper-dual numbers in the area of thermodynamics.

The phase field approach described above was implemented in previous work using finite element method [Die16a, Die17, Die18a]. This is numerically demanding in several aspects. For instance, the conservation of mass has to be guaranteed within the calculation volume. In the literature, several approaches for this are described. Both a penalty-method [Die16a] and a formulation based on Lagrange multipliers [Die17] was employed successfully to tackle this problem. For the implementation of the Lagrange multiplier method a global constraint had to be implemented in the finite element formulation. For this, the source code of the finite element program FEAP (Finite Element Analysis Program) was adapted. The method was developed and tested for 2D simulations first and then extended to 3D simulations. Based on an evolution equation, droplets are relaxed toward the static equilibrium. Special attention was given to the choice of a suitable stopping criterion for the evolution equation upon reaching static equilibrium. In order to ensure a minimal free energy, a stability analysis is necessary. Using an eigenvalue analysis of the system matrix, the stationary solutions were assessed concerning their stability [Die18a]. The same holds true for DGT for which such analysis has not been applied before to the best of our knowledge.



(a) (b)

**Figure 2:** Three-dimensional phase field simulation: (a) droplet on cylinder: initial state (left) and equilibrium state (right). (b) Droplet on structured surface (equilibrium state). The total mass is conserved with the Lagrange-multiplier method. The contact angle between droplet and surface is visible [Die17].

With the help of the phase field model, the static wetting behaviour of structured surfaces was investigated. The simulations allow predictions of the wetting behaviour of several relevant surfaces. Structures investigated are e.g. grooves, truncated pyramids or cylinders, see figure 2.

In addition to prior work on static wetting and adsorption, preliminary work has been done in CRC 926 on phase field modelling of dynamic wetting. First phase field and molecular simulations were performed for moving droplets, which showed that the phase field model is extendable to dynamic wetting scenarios.

In a dedicated preliminary study for the present project proposal it was shown that the present version of our phase field simulation code is able to describe a droplet detachment from a wall. Preliminary results are shown in figure 3. It illustrates the influence of a horizontal vibration with varying frequency on the shape of a hanging droplet and the motion of its centre of mass. The simulation serves as a proof of concept for the simulation tool. No physical interpretation of the results was intended.

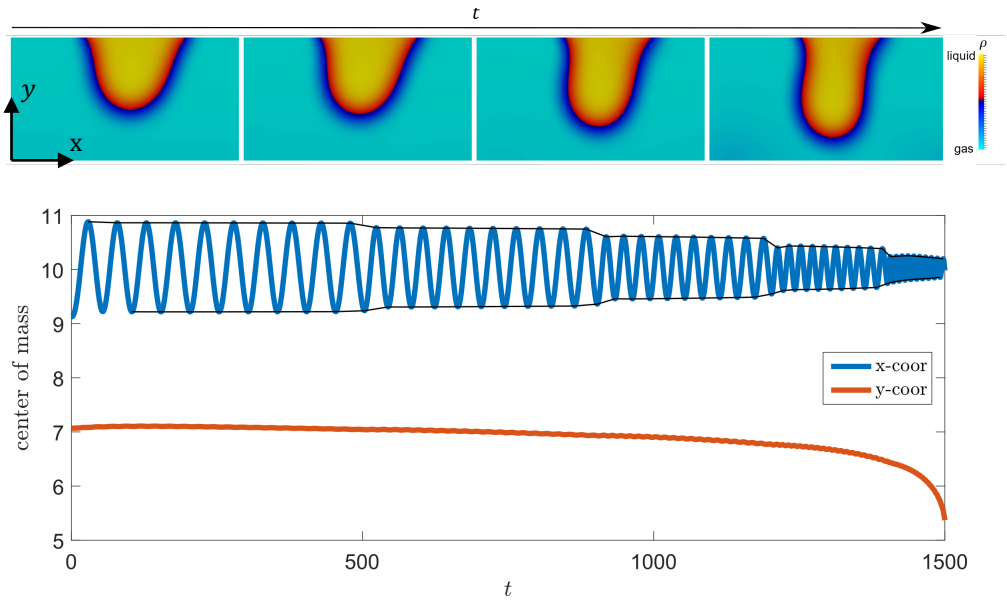



**Figure 3:** Dynamic phase field simulations of droplet detachment. A droplet is hanging on a substrate which is vibrating horizontally with increasing frequency. The contour plots at the top show snap shots of the density distribution. The graph at the bottom shows the time evolution of the centre of mass of the computational domain. Quantities are nondimensionalized by LJ units.

In CRC 926, also the dynamic wetting of droplets hitting a surface is investigated experimentally. A setup for 3D high-speed imaging of a collision process was developed to examine impact of fine solid or liquid particles on a fixed surface [Kru18]. The setup in figure 4 consists of three synchronized high-speed cameras coupled with the microscope lens to capture fine particles and droplets (> 30 µm with a resolution of 700 nm/px) and resolve their contact line with a surface during collision. The dynamic contact angle, movement of the contact line and droplet shape can be obtained with an in-house written MATLAB-script, see figure 4. Additionally, a piezoelectric droplet generator was developed, which can dispense a minimum volume of ten nanoliter (250 µm diameter) of several different liquids like water, methanol and toluene.

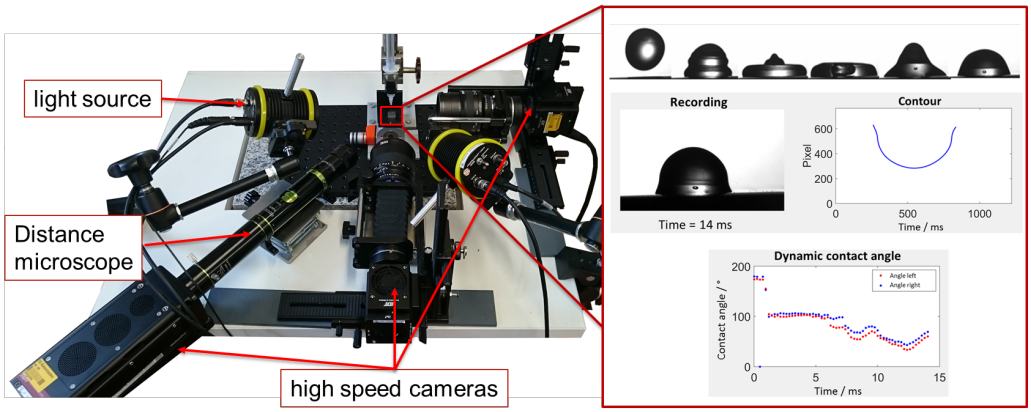



**Figure 4:** Experimental setup for particle or droplet collision with the stationary surface (left); High-speed recording of the droplet collision (right top); shape of the droplet in a current position (right middle) and time-dependent dynamic contact angle during collision (right bottom).

Furthermore, the adhesion of fine solid particles on different substrates was studied experimentally using the vibration method [Hart11], which is based on the detachment of micrometer sized solid particles from a vibrating surface. Using a piezo-driven vibration generator the substrate and therefore the particles are accelerated. If the inertia force due to this acceleration of the substrate overcomes the adhesion force the particle detaches from the surface. The substrate movement is adjusted by a function generator with a variation of the amplitude and frequency from 1 mHz up to 24 kHz. The acceleration and amplitude of the substrate was monitored during the experiments with a laser Doppler vibrometer (Polytec) mounted on a microscope. The particle detachment was detected using a reflected light microscope.

In a preliminary feasibility study for the present project, it was shown that with the existing equipment also the detachment of liquid droplets from a vibrating surface can be studied. It is anticipated that in the experiments of the present project parameters like the temperature and the humidity will play will play a role. They are controlled in the experimental setup.

Furthermore, in other preliminary work in CRC 926 the influence of the surface cleaning procedure on the wetting on chemically pure titanium and technical steel [Bec16a] was investigated. In recent follow-up work, in which also gold substrates were used, it was shown that the result for the contact angle depends mainly on the composition of the organic layer that is adsorbed on the surface of the substrate. This composition, in turn, depends on the nature of the substrate, the cleaning procedure, and the handling of the sample.

## 1.1 Project-related publications

### 1.1.1 Articles published by outlets with scientific quality assurance, book publications, and works accepted for publication but not yet published.

[Bec16a] S. Becker, R. Merz, H. Hasse, M. Kopnarski: Solvent cleaning and wettability of technical steel and titanium surfaces, Adsorpt. Sci. Technol. 24 (2016) 261-274. DOI: 10.1177/0263617416645110.
[Bec17] S. Becker, M. Kohns. H. M. Urbassek, M. Horsch, H. Hasse: Static and Dynamic Wetting Behavior of Drops on Impregnated Structured Walls by Molecular Dynamics Simulation, J. Phys. Chem. C 121 (2017) 12669-12683. DOI: 10.1021/acs.jpcc.6b12741.
[Die16a] F. Diewald, C. Kuhn, R. Blauwhoff, M. Heier, S. Becker, S. Werth, M. Horsch, H. Hasse, R. Müller: Simulation of Surface Wetting by Droplets Using a Phase Field Model, Proc. Appl. Math. Mech. 16 (2016) 519-520. DOI: 10.1002/pamm.201610248.

[Die17] F. Diewald, C. Kuhn, M. Heier, M. Horsch, K. Langenbach, H. Hasse, R. Müller: Surface Wetting with Droplets: A Phase Field Approach, Proc. Appl. Math. Mech. 17 (2017) 501-502. DOI: 10.1002/pamm.201710220.
[Die18a] F. Diewald, C. Kuhn, M. Heier, K. Langenbach, M. Horsch, H. Hasse, R. Müller: Investigating the stability of the phase field solution of equilibrium droplet configurations by eigenvalues and eigenvectors, Comput. Mater. Sci. 141 (2018) 185-192. DOI: 10.1016/j.commatsci.2017.08.029.
[Die18b] F. Diewald, M. Heier, M. Horsch, C. Kuhn, K. Langenbach, H. Hasse, R. Müller: Three-Dimensional Phase Field Modeling of Inhomogeneous Gas-Liquid Systems Using the PeTS Equation of State, J. Chem. Phys. 149 (2018) 064701. DOI: 10.1063/1.5035495.
[Har11] J. Hartmüller, S. Ripperger: Untersuchung der Haftung von kugelförmigen Glaspartikeln an technischen Oberflächen mit der Vibrationsmethode. Chemie Ingenieur Technik 84 (2011) 100-107. DOI:10.1002/cite.201100099
[Hei18a] M. Heier, S. Stephan, J. Liu, W. G. Chapman, H. Hasse, K. Langenbach: Equation of state for the Lennard-Jones truncated and shifted fluid with a cut-off radius of 2.5 σ based on perturbation theory and its applications to interfacial thermodynamics, Mol. Phys. 116 (2018) 2083-2094. DOI: 10.1080/00268976.2018.1447153.
[Kru18] F. Krull, R. Hesse, P. Breuninger, S. Antonyuk: Impact behaviour of microparticles with microstructured surfaces: Experimental study and DEM simulation, Chemical Engineering Research and Design 135 (2018) 175-184. DOI: 10.1016/j.cherd.2018.05.033
[Wer16b] S. Werth, M. Kohns, K. Langenbach, M. Heilig, M. Horsch, H. Hasse: Interfacial and bulk properties of vapor-liquid equilibria in the system toluene + hydrogen chloride + carbon dioxide by molecular simulation and density gradient theory + PC-SAFT, Fluid Phase Equilib. 427 (2016) 219-230. DOI: 10.1016/j.fluid.2016.07.016.

#### 1.1.2 Other publications
None

#### 1.1.3 Patents
None

## 2 Objectives and work programme

### 2.1 Anticipated total duration of the project

First funding period (this proposal): 3 years, starting October 2019

### 2.2 Objectives

The aim of the project is to gain a fundamental physical understanding of the complex phenomena that occur during the detachment of droplets from vibrating surfaces. With this focus the project is perfectly embedded in SPP 2171: Droplet detachment is an important de-wetting process, the switching of the surface is established here by the control of its movements, e.g. by ultrasonic waves. The goal of the project is reached by a combination of different simulation and experimental methods. Not only qualitative knowledge but also quantitative descriptions will be obtained.

The detachment of droplets from vibrating surfaces is influenced by many parameters: Inertia, viscosity, surface tensions (liquid-gas, liquid-solid, gas-solid), and external fields (namely gravity) to name only the most obvious ones. These effects act in scenarios that are characterized by geometric parameters like the size of the droplet, the modes of the movement of the surface, and the conditions like temperature. Furthermore, the nature of the fluid and the solid as characterized by the different relevant material properties are of utmost importance.

For describing the influence of different parameters on complex phenomena like the de-wetting of vibrating surfaces, the individual parameters can be advantageously combined to dimension-less numbers. This approach reduces the dimensionality of the parameter space that has to be investigated.

The detachment of the droplet from the surface can take place in different ways, e.g. one or more droplets may be ejected, parts of the droplet may remain on the surface or not. The project aims at gaining insight into the influence of different parameters on the detachment mechanism of droplets. Some central questions that shall be addressed in the project are:

- What is the influence of dynamic excitation of the surface, such as frequency, amplitude, and modes of movements?
- What is the influence of fluid and solid properties, such as density, viscosity, surface tension, and contact angle?
- What is the difference in excitation modes, such as translation in horizontal and vertical direction versus rotational excitation?
- What is the mechanism of detachment: Detachment as a connected droplet, fragmentation into two or more droplets, residual liquid on the surface?
- Can we find dimensionless numbers that describe the influence of relevant input parameters and related mechanism?

In the first funding period, we will treat the substrate as rigid and simply prescribe its movement. In the second funding period we want to take surface deformation due to interaction with the liquid and the dynamic excitation (wave propagation) into account. Furthermore, in the first funding period only smooth surfaces will be considered. The studies may be extended to rough surfaces in the second funding period.

### 2.3 Work programme including proposed research methods

In the project, an interdisciplinary multiscale approach is applied to reach the goals described above. On the nanoscale molecular dynamics simulations will be used to study the detachment of nanosized droplets from surfaces. On the meso- and macroscale a phase field approach in combination with a finite element method will be used. Both approaches are linked by an equation of state in combination with thermodynamic density gradient theory (DGT). All studies of the present work will be carried out at isothermal conditions.

The phase field method enables the simulation of droplets that can also be observed in experiments. The visual observations in the experiments provide lateral and horizontal images of the detachment process from a dynamically moving substrate. Not only harmonic oscillations (both parallel and perpendicular to the normal vector on the substrate surface) will be considered but also other modes of movement e.g. pulse-like excitations. In the experiments, different liquids and substrates will be used, namely: water, ethanol, and cyclohexane on gold, titanium, and polyethylene. The cleaning of the surface is expected to play a role. Here, we can build on extensive preliminary work on the influence of cleaning procedures on the contact angles and the surface contamination, see above.

In order to obtain a fundamental understanding of the underlying physics all groups will cooperate to develop a set of relevant dimensionless numbers that characterize the droplet detachment process. This will be achieved by a synergetic view on the multiscale simulations and experimental observations.

The research is organized in five work packages which are described in the following.

Work package 1: Molecular dynamics simulations

Molecular dynamics simulations of the detachment of nanosize droplets from walls will be performed for dispersive systems in which a LJTS fluid is in contact with a wall that is also described by LJTS sites. In designing these studies we can build on comprehensive knowledge that was acquired in the preliminary work on this type of systems. The relevant parameters (including molecular parameters like the attraction between the wall and the fluid) will be varied systematically, the resulting modes of detachment of a droplet will be determined and quantitative data on the detachment process will be collected. External forces will be applied to the wall atoms to induce the desired modes of movement of the wall. In preliminary studies the influence of the system size on the results will be investigated. We expect that due to the excellent parallel performance of the simulation code, systems sizes can be reached for which fluctuations, like those of the droplet form, have only a minor influence on the results. This is the prerequisite for a direct comparison with the results from the phase field simulations, which do not account for these fluctuations. The comparison between the results from the molecular simulations and the phase field simulations will also reveal whether or not it is necessary to attribute special features to the three phase line for describing the studied process with continuum theories. We emphasize that the molecular simulations and the phase field simulations of the systems discussed here are thermodynamically consistent in the sense that all relevant thermodynamic properties are the same in both methods.

For the dispersive LJTS model systems, the corresponding phase field model is already available from previous work. However, this is not the case for the systems that will be studied experimentally and for which phase field simulations shall be carried out too. The corresponding fluids will be modelled by an equation of state based on molecular thermodynamics which is provided in the present work package. The liquid-vapour surface tension will be included as described above using DGT. The substrates and their interactions with the fluid will be described in a first step based on contact angle measurements that are carried out in the present project with existing equipment. The challenge of the influence of the cleaning of the surfaces on the results will be given special attention based on the experience gained in our previous studies.

It is not planned to develop atomistic models for the nine systems that shall be studied experimentally. This would require an effort which is out of the scope of the present work package. If time allows, some preliminary atomistic simulation studies on one or two of the systems that are studied experimentally will be carried out.

Work package 2: Phase field simulations

The thermodynamic information is incorporated into the phase field model via the free energy of the system as described above using the method of hyper-dual numbers, which allows for automatic differentiation. For solving the equations of the phase field model, a mixed finite element method (Q2-P1-formulation) is used. In addition to the constitutive modelling of the liquid, the surface will be introduced as rigid solid. This induces the challenge that an Eulerian description using the velocity field has to be combined with a Lagrangian type formulation of the boundary conditions. The surface of the solid is discretized by special surface elements that enforce the contact angle condition.

With regard to excitation, different time signals are to be investigated. This includes harmonic zigzag, and Heaviside excitations. Being an important parameter, the frequency will be varied. It

is suspected that the droplet motion resembles a damped non-linear oscillator. Thus an amplitude dependency is likely to be relevant and will be investigated by performing frequency up and down sweeps.

For the dispersive LJTS systems, direct comparisons of the results of the phase field simulations and the molecular dynamics simulations will be performed. The droplet motion in both types of simulation will be compared. For the phase field simulation the interfaces need special attention, as in this region strong field gradients (density) appear. In order to resolve them properly a fine mesh is required. If it renders necessary, adaptive strategies will be used to refine the mesh in the transition layer between liquid and gas.

The phase field model is then scaled up to be able to simulate large length scales. In this respect the transition layer has to be broadened without changing its thermodynamic properties, i.e. surface tension. This enables meso- and macroscale simulations which can be compared to experimental results. This upscaling has to be done carefully. Numerical tests concerning the static equilibrium shapes will be performed to verify that thermodynamic properties of the liquid as well as contact conditions are not changed unintentionally by the upscaling step. Subsequently, dynamic runs will be performed to simulate the detachment of droplets of on the large scales. The influence of relevant parameters will be investigated. Again these include the influence of frequency and amplitude of the excitation. These simulations are the basis for a comparison to experimental investigations, which are in the focus of the next work package.

Work package 3: Experimental investigations

The physical mechanisms of de-wetting and the detachment of small droplets from dynamically activated surfaces will be studied experimentally by a combination of the vibration method with the three-dimensional high-speed imaging. The water, ethanol, and cyclohexane droplets on the gold, titanium, and polyethylene surfaces will be investigated The droplet motion on a vibrating surface is observed with three synchronised high-speed cameras with a resolution of 700 nm/px and 1600x1200 px with 9300 fps, see figure 5. The cameras are arranged horizontal and vertical to the substrate to measure the droplet shape and contact angle. Additionally, a climatic chamber will be constructed to ensure a constant temperature and humidity during the experiments.

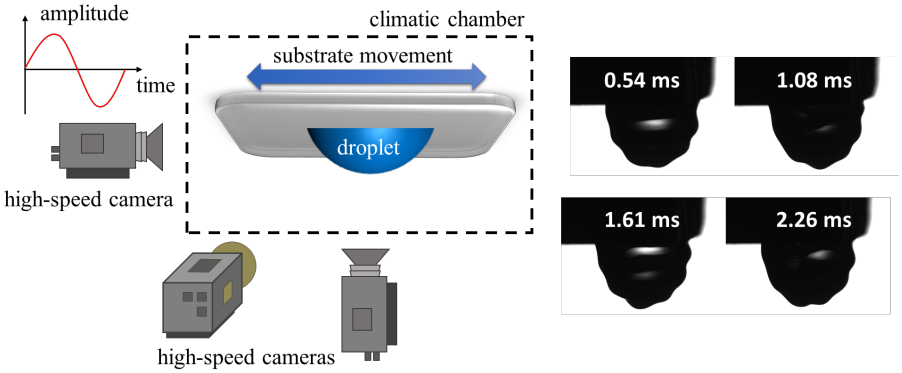



**Figure 5:** Sketch of the experimental setup to investigate the droplet detachment mechanism (left). High-speed recording during a preliminary test of water droplet (6 µl) on a horizontally vibrating surface at 440 Hz (right).

At the beginning of the experiment, a single droplet will be generated and placed on the substrate. In order to produce single fine droplets (< 10 nanoliter) with a defined liquid volume of water, ethanol, or cyclohexane the nozzle of the droplet generator will be functionalized to improve the droplet ejection. This functionalization can be performed in cooperation with the

project of Dr. Vollmer (MPI Mainz). After the wetting of the surface, firstly the equilibrium shape of the droplet and the static contact angle will be measured. It is known that the contact angle is primarily influenced by the properties and conditions of the substrate in the direct vicinity of the surface. Therefore, a special consideration is given to the cleaning and preparation of the surface. Once static wetting properties are in agreement to simulation results, the dynamic de-wetting by droplet detachment is analysed. During the experiments, the time signal of the oscillation (frequency, amplitude) will be varied. The variation of the amplitude range (from micrometre to millimetre) will be realized by using different kind of vibrations stimulators like piezo-driven and electrodynamic generators. A function generator will be used to adjust the frequency and the waveform arbitrarily (e.g. sine or square pulse). The droplet–surface behaviour captured in 3D by high-speed-imaging provide the important knowledge about the dynamical change of the contact line, shape and contact angle of the droplet.

Work package 4: Validation

During the entire project, the comparison and validation of the results that were obtained with the different methods is always in the focus. Therefore, a special work package is devoted to this task. The results from the systematic studies of the dispersive systems by atomistic simulations and by phase field simulations can be compared directly as they are based on the same thermodynamics. On the one hand, this contributes to the validation of both methods. On the other hand, this enables identifying the scale-dependent influence of effects like fluctuations and adsorption on the wall, which are only accounted for in the atomistic simulations, on the results.

A challenge in the comparison of molecular dynamics simulations to phase field simulations lies in the stochastic character of the molecular dynamics method. As fluctuations are not present in the continuum approach by the phase field method, proper averages have to be introduced in comparison. This will include for example the motion of the centre of mass of a droplet in both methods.

On the other hand, the phase field results will be compared to experimental results. Again, this contributes to the validation of the phase field model, including the assumptions that have to be made for describing real systems, e.g. regarding the solid-fluid interactions. A prerequisite for the comparison of the results for the dynamic de-wetting processes obtained by experiment and by the model is that the static contact angle is consistently described. Using image processing and motion tracking techniques the experimental observations will be analysed to identify the type and instant of droplet detachment. These characteristics are again compared to simulation results.

Work package 5: Physical insights and quantitative descriptions by dimensionless numbers

The main goal of the project is to obtain a fundamental understanding of the complex processes that occur during droplet detachment from vibrating surfaces. A large body of data will be generated in the project with different methods. These data differ not only in the way they were obtained (molecular simulation, phase field simulation, experiment) but also in their type. In the studies of the dispersive model systems, in principle all parameters that influence the process can be varied systematically (within the limits given by the available computational resources). This is ideal for establishing correlations of the studied phenomena, like the conditions for the droplet detachment or the conditions for the detachment of a single droplet without fragmentation. In a first step, the parameters that govern the process need to be identified and

combined in some suitable way to dimensionless parameters. There is no unique way to do this and several choices will be explored in the project. The knowledge of these dimensionless parameters helps also to design the programs for the computer experiments and the laboratory experiments. The number of experiments that are needed to suitably explore a given parameter space can be drastically reduced without losing information if only the dimensionless parameters are varied but not the usually much higher number of parameters that carry dimensions.

These considerations will also lead to a deep understanding of the interplay of the different parameters that govern the detachment of droplets from vibrating surfaces. Also the rich phenomenology of the possible ways in which this detachment can occur will be explored. This last work package strongly relies on the cooperation of the different disciplines (thermodynamics, continuum mechanics, experimental mechanical process engineering).

All five work packages will mostly run in parallel over most of the project's duration.

### 2.4 Data handling

The findings, the simulation results as well as the experimental results will be reported in scientific publications in international journals. Primary data from the simulations and the experiments will be stored for at least 10 years. If appropriate, extended results like movies will be deposited in electronic form as supplementary material in the journals.

All results will also be made available in a freely accessible form in the engrXiv repository in agreement with the provisions of the German § 34 UrhG.

### 2.5 Other information

There is no overlap of the work that is to be carried out in the present project with any work that is carried out or planned by the applicants within CRC 926. However, strong synergetic effects would be created if both projects could be carried out as planned.

Interactions with other projects within SPP 2171 can be described presently only in a general manner, as it is not known which projects will be funded. All projects will share a common interest in dynamic wetting/de-wetting and in the control of the processes by switchable surfaces. This is also at the heart of the present project proposal. Furthermore, the methodological scope of the present project is wide and spans from atomistic simulations over continuum simulations to experiments. There is hence reason to believe that there will also be an important overlap in the methodological interests with other projects of SPP 2171. We are confident that the present project will profit strongly from the environment of SPP 2171 and that it will also contribute to other projects in SPP 2171.

Three of the four applicants have already participated successfully in several SPP programs (in two cases also as speaker), the fourth applicant is a young scientist who would gain experience. All applicants have co-operated closely in other projects.

### 2.6 Descriptions of proposed investigations involving experiments on humans, human materials or animals as well as dual use research of concern

None.

## 2.7 Information on scientific and financial involvement of international cooperation partners

None.

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# 4 Requested modules/funds

Funds are basically only requested for personnel and travel. The equipment that is needed for the experimental studies and the simulations is available. To carry out the project, two PhD students are required. One of them will carry out the phase field simulations and will be assigned to the Institute of Applied Mechanics. The other one will carry out the experiments and the molecular simulations. His position is assigned here formally 50% to the Institute of Particle Process Engineering and 50% to the Institute of Thermodynamics. It is planed to hire highly qualified candidates from engineering. This requires a full position (100%).

***Müller, Ralf (Institute of Applied Mechanics, University of Kaiserslautern)***

## 4.1 Basic Module

### 4.1.1 Funding for Staff

The phase field simulations will be carried out by a PhD student with a background in continuum mechanics. A sound knowledge in numerical methods and programming is required to deal with the necessary implementations and to perform the studies.

100% PhD student for 3 years 193,500 EUR

A student researcher will support the work within the project. The student researcher will perform parameter studies and support the PhD student in testing implementations and in post-processing of simulation data.

Student researcher without university degree for 3 years, 10h/week 15,600 EUR

### 4.1.2 Direct Project Costs

None.

#### 4.1.2.1 Equipment up to Euro 10,000, Software and Consumables

The new version 8.5 of the finite element programme FEAP (Finite Element Analysis Program) will be used within the project. For previous versions of the programme many extensions have been developed at the Institute of Applied Mechanics, such as parallel solvers, GPU-based

solvers, and visualization interfaces by ParaView, TECPLot and VisIt. These extensions can be exported to the new version.

FEAP 8.5 1,500 EUR

#### 4.1.2.2 Travel Expenses

The PhD student and applicant will travel to the meetings and workshops within the Priority Programme 2171 (2,000 EUR). Furthermore, the results will be presented at two international conferences (2,000 EUR).

4,000 EUR

#### 4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

None.

#### 4.1.2.4 Expenses for Laboratory Animals

None.

#### 4.1.2.5 Other Costs

None.

#### 4.1.2.6 Project-related publication expenses

None.

### 4.1.3 Instrumentation

#### 4.1.3.1 Equipment exceeding Euro 10,000

None.

#### 4.1.3.2 Major Instrumentation exceeding Euro 50,000

None.

***Hasse, Hans and Langenbach, Kai (Institute of Thermodynamics, University of Kaiserslautern)***

## 4.1 Basic Module

### 4.1.1 Funding for Staff

The molecular simulations and the development of the thermodynamic models for the systems that are studied experimentally shall be carried out by a PhD student with a sound knowledge of thermodynamics.

50% PhD student for 3 years 96,750 EUR

The student researcher will perform parametric runs for the molecular dynamics simulations and support the PhD student in the post-processing of simulation data.

Student researcher without university degree for 3 years, 5h/week 7,800 EUR

#### 4.1.2 Direct Project Costs

None.

##### 4.1.2.1 Equipment up to Euro 10,000, Software and Consumables

None.

##### 4.1.2.2 Travel Expenses

The PhD student and the applicants will travel to the meetings and workshops within the Priority Programme 2171 (1,500 EUR). Furthermore, the results are presented at an international conference (1,000 EUR).

2,500 EUR

##### 4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

None.

##### 4.1.2.4 Expenses for Laboratory Animals

None.

##### 4.1.2.5 Other Costs

None.

##### 4.1.2.6 Project-related publication expenses

#### 4.1.3 Instrumentation

##### 4.1.3.1 Equipment exceeding Euro 10,000

None.

##### 4.1.3.2 Major Instrumentation exceeding Euro 50,000

None.

***Antonyuk, Sergiy (Institute of Particle Process Engineering, University of Kaiserslautern)***

### 4.2 Basic Module

#### 4.2.1 Funding for Staff

The experimental investigations of de-wetting require a PhD student with a sound knowledge of experimental methods, data acquisition, and image processing.

50% PhD student for 3 years 96,750 EUR

A student researcher will support the work within the project. The student researcher will assist in setting-up and performing the experiments. Furthermore, the student researcher will support the PhD student in post-processing the image data obtained during the experiments.

Student researcher without university degree for 3 years, 5h/week 7,800 EUR

#### 4.2.2 Direct Project Costs

None.

##### 4.2.2.1 Equipment up to Euro 10,000, Software and Consumables

Consumables for the experiments, such as surface materials and liquids, cleaning materials are needed. To store the image data during the experimental investigations additional storage media are required.

Base material, liquids, cleaning, data storage 1,000 EUR

##### 4.2.2.2 Travel Expenses

The PhD student and applicant will travel to the meetings and workshops within the Priority Programme 2171 (1,000 EUR). Furthermore, the results are presented at an international conference (1,000 EUR).

2,000 EUR

##### 4.2.2.3 Visiting Researchers (excluding Mercator Fellows)

None.

##### 4.2.2.4 Expenses for Laboratory Animals

None.

##### 4.2.2.5 Other Costs

None.

##### 4.2.2.6 Project-related publication expenses

#### 4.2.3 Instrumentation

##### 4.2.3.1 Equipment exceeding Euro 10,000

None.

##### 4.2.3.2 Major Instrumentation exceeding Euro 50,000

None.

## 5 Project requirements

### 5.1 Employment status information

- Müller, Ralf, Prof. Dr.-Ing. habil.: Permanent position (W3)
- Hasse, Hans, Prof. Dr.-Ing. habil.: Permanent position (W3)
- Langenbach, Kai, Jun. Prof.: Temporary position (W1), limited till 02nd July 2020, further employment until 2nd July 2023 intended
- Antonyuk, Sergiy, Prof. Dr.-Ing.: Permanent position (W3)

### 5.2 First-time proposal data

None.

### 5.3 Composition of the project group

Both PhD students will co-operate closely on a day-to-day basis. Their offices will be in the same building on the same floor. The PhD students will be supervised by the team of four project leaders with the following foci:

- Müller, Ralf: Phase field simulations
- Hasse, Hans: Molecular simulations
- Langenbach, Kai: Equations of state, DGT, DFT
- Antonyuk, Sergiy: Experiments

Additional support will be provided from Jun. Prof. Dr.-Ing. Charlotte Kuhn (Institute of Applied Mechanics, phase field simulations) and Jun. Prof. Dr.-Ing. Maximilian Kohns (Institute of Thermodynamics, molecular simulations). Daniel Fröscher (Institute of Thermodynamics, IT Specialist) assists in performing the simulations. Dr.-Ing. Kai Nikolaus (Institute of Particle Process Engineering, experiments) and Dipl-Ing. (FH) Denis Goldnik, (Institute of Particle Process Engineering, experiments) help in performing the experimental investigations.

### 5.4 Cooperation with other researchers

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

The project team will cooperate with Prof. Walter Chapman, Rice University, Houston, Texas, USA with regard to DGT and DFT,

Cooperation with the project of Vollmer/Schmid (Max Planck Institute for Polymer Research, Mainz): For the experimental study of droplet detachment by vibration (WP3), a new generator for very small single droplets must be developed. This will be realized by coating the dosage needle with a super-hydrophobic layer in cooperation with the project of D. Vollmer. She has a lot of experience in preparing super liquid repellent layers. In addition, in our project, the dynamic wetting behavior of droplets will be compared with measurements with confocal microscopy performed by D. Vollmer.

Cooperation with the project of Auernhammer (Leibniz Institute of Polymer Research Dresden): We will perform experiments on vibrating substrates from the group of Auernhammer to characterize the effect of mechanical excitation on the contact angle hysteresis.

The excitation of the droplets can be achieved with an alternative method, which is used in the project of Schönecker and Oesterschulze (University of Kaiserslautern). This project will provide us the surfaces with electrodes. By applying the alternating voltage, the droplets are excited and their dynamic de-wetting behaviour on these substrates is investigated in WP3 of this project. For the project of Schönecker/Oesterschulze, we will provide the distance microscopes to increase the imaging resolution by the capturing of the contact line.

The knowledge on the dynamical change of droplet shape and the contact line during vibration obtained in this project by the high-speed imaging is complimented by important information about the fluid dynamics inside the droplet. These data will be obtained by astigmatism-PTV (Particle Tracking Velocimetry) technique used in project of Hussong and Gurevich (Ruhr-Universität Bochum). The vibration setup of Kaiserslautern will be transported to Bochum to perform the measurements under the same conditions.

The high-speed imaging setup developed in this project can be used in the project of Gambaryan-Roisman (Technische Universität Darmstadt) to determine the spreading and

evaporation dynamics of micrometer sized droplets on the deformable structured surfaces or surfaces with porous coating.

The simulation tool on the basis of the multiscale approach (molecular dynamics simulations and phase field approach) developed in this project can be used in other projects of SPP 2171 for the simulation of dynamical wetting behavior, for example in the project of Huber (University of Hamburg) for dynamical wetting of electrically conductive nano porous substrates.

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

Prof. Jörg Schröder, University Duisburg-Essen, Germany
Prof. Tarek Zohdi, University of California at Berkeley, Berkeley, California, USA
Prof. Baixiang Xu, TU Darmstadt, Germany
Prof. Bob Svendsen, RWTH Aachen, Germany
Jun. Prof. Marc-André Keip, University of Stuttgart, Germany
Prof. Franz-Dieter Fischer, University of Leoben, Austria
Prof. Jakob Burger, TU München, Germany
Dr. Martin Horsch, STFC Daresbury Laboratory, UK
Prof. Jadran Vrabec, TU Berlin, Germany
Prof. Sabine Enders, KIT, Germany
Prof. J.A.M. Kuipers, University of Eindhoven, Netherlands
Prof. J. D. Litster, Sheffield University, UK
Prof. U. Bröckel, Umwelt-Campus Birkenfeld, Germany
Prof. V. Schmidt, Universität Ulm, Germany
Prof. M. Thommes, TU Dortmund, Germany
Prof. S. Heinrich, Hamburg University of Technology, Germany

## 5.5 Scientific equipment

The equipment that is needed for the experimental studies is available (repurchase value more than 400,000 EUR). The same holds for the computational resources. Phase field simulations are routinely carried out on a Linux Cluster (laplace: 12 compute-nodes, 260 cores, including GPU-nodes). For larger phase field simulations and the molecular simulations computational resources of RHRK Kaiserslautern (a member of Gauss Allianz) as well as of the National High Performance Computing Centres in Stuttgart and Munich are used, to which the applicants have access.

## 5.6 Project-relevant cooperation with commercial enterprises

None.

## 5.7 Project-relevant participation in commercial enterprises

None.

# 6 Additional information

None.