## Systematic Molecular Dynamics Simulation Study of Adsorption and Contact Angles in Dispersive Systems

Michaela Heier<sup>C, S</sup> and Martin Horsch

Laboratory of Engineering Thermodynamics, University of Kaiserslautern, Kaiserslautern, Rheinland-Pfalz, Germany michaela.heier@mv.uni-kl.de

Felix Diewald

Institute of Applied Mechanics, University of Kaiserslautern, Kaiserslautern, Rheinland-Pfalz, Germany

Kai Langenbach

Laboratory of Engineering Thermodynamics, University of Kaiserslautern, Kaiserslautern, Rheinland-Pfalz, Germany

Ralf Müller

Institute of Applied Mechanics, University of Kaiserslautern, Kaiserslautern, Rheinland-Pfalz, Germany

## Hans Hasse

Laboratory of Engineering Thermodynamics, University of Kaiserslautern, Kaiserslautern, Rheinland-Pfalz, Germany

Both the contact angle of a droplet on a wall and the adsorption of the fluid at the wall depend on the fluid-wall interactions. For dispersive systems, we have recently carried out a systematic molecular dynamics study which has yielded quantitative information on the dependence of the macroscopic contact angle on the temperature and the strength of the fluid-wall interaction [1]. That study is extended here to adsorption, so that a comprehensive quantitative picture of both wetting and adsorption in dispersive systems is obtained. The studied system consists of Lennard-Jones truncated and shifted (LJTS) sites which are used both for representing the fluid and the wall. It is shown in [1] that the results are generic and also hold for other dispersive systems. The adsorption from gas and supercritical phases on the wall is studied. Adsorption isotherms are determined for temperatures from the triple point up to three times the critical temperature of the fluid. The strength of the fluid-wall interaction is systematically varied and chosen such that the resulting contact angles range between 0° and 180°, i.e. total wetting and no wetting. For temperatures below the critical temperature of the fluid, upon increasing the pressure first monolayer and then multilayer adsorption is observed, as expected. In cases in which the contact angle  $\Theta$  between the liquid and the wall is above 0°, upon increasing the pressure, finally droplets form at the wall. In these cases (and only then), also metastable states are observed: the adsorption isotherms can be extended above the vapor pressure of the fluid without the occurrence of condensation. In all cases with total wetting ( $\Theta = 0^{\circ}$ ) the maximum pressure is always the vapor pressure of the fluid and the surface excess shows a singularity at that pressure due to condensation on the flat fluid surface. For temperatures above the critical temperature of the fluid, droplet formation is no issue and all adsorption isotherms are similar and show the expected dependencies.

References:

[1] S. Becker, H.M. Urbassek, M.T. Horsch, H. Hasse: Contact Angle of Sessile Drops in Lennard-Jones Systems, Langmuir, 30 (2014) 13606 - 13614.