Abstract Submitted
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Droplets and the three-phase contact line at the nano-scale. Statics and dynamics PETR YATSYSHIN, DAVID SIBLEY, Imperial College London, NIKOS SAVVA, Imperial College London; Cardiff University, SERAFIM KALLIADASIS, Imperial College London — Understanding the behaviour of the solid-liquid-vapour contact line at the scale of several tens of molecular diameters is important in wetting hydrodynamics with applications in micro- and nano-fluidics, including the design of lab-on-a-chip devices and surfaces with specific wetting properties. Due to the fluid inhomogeneity at the nano-scale, the application of continuum-mechanical approaches is limited, and a natural way to remedy this is to seek descriptions accounting for the non-local molecular-level interactions. Density Functional Theory (DFT) for fluids offers a statistical-mechanical framework based on expressing the free energy of the fluid-solid pair as a functional of the spatially varying fluid density. DFT allows us to investigate small drops deposited on planar substrates whilst keeping track of the microscopic structural details of the fluid. Starting from a model of intermolecular forces, we systematically obtain interfaces, surface tensions, and the microscopic contact angle. Using a dynamic extension of equilibrium DFT, we investigate the diffusion-driven evolution of the three-phase contact line to gain insight into the dynamic behaviour of the microscopic contact angle, which is still under debate.

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