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Computing fluid-particle interaction forces for nano-suspension droplet spreading: molecular dynamics simulations WEIZHOU ZHOU, BAIOU SHI, EDMUND WEBB, Lehigh Univ — Recently, there are many experimental and theoretical studies to understand and control the dynamic spreading of nano-suspension droplets on solid surfaces. However, fundamental understanding of driving forces dictating the kinetics of nano-suspension wetting and spreading, especially capillary forces that manifest during the process, is lacking. Here, we present results from atomic scale simulations that were used to compute forces between suspended particles and advancing liquid fronts. The role of nano-particle size, particle loading, and interaction strength on forces computed from simulations will be discussed. Results demonstrate that increasing the particle size dramatically changes observed wetting behavior from depinning to pinning. From simulations on varying particle size, a relationship between computed forces and particle size is advanced and compared to existing expressions in the literature. High particle loading significantly slowed spreading kinetics, by introducing tortuous transport paths for liquid delivery to the advancing contact line. Lastly, we show how weakening the interaction between the particle and the underlying substrate can change a system from exhibiting pinning behavior to de-pinning.

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