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Dynamic Contact Angle at Nano-Scale: a Unified View

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Dynamic Contact Angle Generation in Liquid Flow

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Generation of dynamic contact angle in the course of wetting is a fundamental phenomenon of nature. Dynamic wetting processes have a direct impact on flows at nano-scale, and therefore their understanding is exceptionally important to emerging technologies. Here, we reveal the microscopic mechanism of dynamic contact angle generation. It has been demonstrated using large-scale molecular dynamics simulations of bead-spring model fluids that the main cause of local contact angle variations is the distribution of microscopic force acting at the contact line region. We were able to retrieve this elusive force with high force accuracy. It has been directly established that the force distribution can be solely predicted on the basis of a general friction law for liquid flow at solid surfaces by Thompson & Troian. The relationship with the friction law provides both an explanation of the phenomenon of dynamic contact angle and a methodology for future predictions. The mechanism is intrinsically microscopic, universal and irreducible, and is applicable to a wide range of problems associated with wetting phenomena.

Keywords: dynamic contact angle; molecular dynamics simulations; nanoscale; nonlinear friction; wetting