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Origin of dynamic contact angle at the nanoscale. ALEX LUKYANOV, ALEXEI LIKHTMAN[1], University of Reading — Generation of a dynamic contact angle in the course of wetting is a fundamental phenomenon of nature. Dynamic wetting processes have a direct impact on flows at the nanoscale, and therefore, understanding them is exceptionally important to emerging technologies. Here, we reveal the microscopic mechanism of dynamic contact angle generation, which is demonstrated using large-scale molecular dynamics simulations of bead-spring model fluids. It has been shown 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 force with high accuracy to understand its nature and its characteristic physical parameters. 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 first formulated by Thompson & Troian on the basis of molecular dynamics simulations of Lennard-Jones liquids. 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.

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