Oral presentation

Wetting dynamics using large scale Molecular Dynamics

By

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Wetting dynamics (i.e. phenomena associated with the contact line motion) are involved into a huge number of natural phenomena (including processes inside living organisms) and technological applications. The flow of rain drops on glass presents a most obvious example which still challenges car windshield makers. In spite of such wide importance of wetting dynamics phenomena, they still are under intense debate, mainly because of their complexity. The fluid motion in the region of the fluids close to the contact line differs from its motion in the bulk of the fluid. The very presence of a contact with a solid often slows down the hydrodynamic fluid motion by several orders of magnitude. To a large extend, wetting dynamics seem to depend on several macroscopic factors like viscosity, surface tensions and substrate roughness. However it also seems to be influenced by the (microscopic) chemical structure of the solid, the local modification of the liquid structure by the solid etc. Up to now, a few theoretical models are in use and seem to be able to describe some contact line dynamics.

Large scale molecular dynamics have been used rather recently to study the details of these dynamics. It is the aim of the talk to review the recent results concerning the dynamics of wetting on different types of substrates: flat surfaces, fibres, pores ... Combining theoretical approach, experimental results and large scale molecular simulations, it will be shown that the dynamics of moving wetting line can be related to several channels of energy dissipation (the friction between the liquid and the solid surface, to the viscous bending of the meniscus, ...). Large scale molecular dynamics allow to validate the existence and properties of these channels.