Interfacial dynamics of simple fluids at the nanoscale: a molecular simulation perspective.

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Despite its wide interest in many applications, modeling accurately the dynamics of two phases (fluid-fluid and fluid-solid) interface still remains quite challenging, even when dealing with simple fluids. This is even more complex when three-phase (fluid−fluid−solid) interface dynamics is dealt with, because of the multi-scale (in time and space) nature of such systems. A possible way to improve our understanding of such systems at the nano-scale is to use molecular dynamics simulations in which the interface dynamics behavior emerges without any a priori. Thus, during the presentation, we will illustrate how molecular dynamics simulations of a nanodroplet moving on a perfectly rigid solid can shed light on some small scales phenomena occurring at interfaces and how such information can be impleted in a macroscale simulator based on a Navier Stokes + Volume of fluid strategy.