Molecular Perspective of Wetting: Simulation and Theory



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Introduction

In our daily life and many of industrial applications, we usually find fluids which interact with solid substrates. Although a lot of researches have been carried out and new developments have been made to understand the wetting phenomena at the macroscopic scale, little is known at the nanoscale due the limitation of the experimental methods. Wetting in general can be defined as the process where three phases which at least two of them are fluids are brought together. In most of the situations, a solid surface is wetted by a liquid in the saturated vapor of the liquid. The vapor interface can be also replaced with an immiscible liquid. The interactions between the solid, liquid and the gas phases at the molecular scale determine how the liquid wet the surface.

We can see wetting phenomena in our daily life for example the rain droplets on the window of car or dispersing the powders in milk for breakfast, and also in different industrial and biological applications. We can name some of the industrial applications such as reducing friction between moving surfaces by using different liquids, lab-on-a-chip systems,[1] coating by polymers to protect surfaces, [2] printing applications [3] and penetration of liquids into porous environments.[4] In different applications where properties of a surface are important, very often it is needed to characterize and control the wetting properties of the surface by a liquid. One way to influence the wetting properties of a surface is by changing the surface chemistry, and substantial research has been carried out to control the wetting characteristics of a surface by functionalizing the surface with different chemical groups. The interaction energy of the surface with the liquid and the vapor can be modified with different polar and non-polar groups.

Methods

The structure and dynamic properties of liquids at solid surfaces have been extensively studied by experimental and theoretical investigations due to their high interest in different applications. The wetting and drying properties of solid surfaces are controlled by the molecular interfacial properties, which in turn are governed by the interfacial intermolecular interactions. The range of the intermolecular interactions is in the order of few nanometers. Such length scales can now be studied with different experimental methods like atomic force microscopy. However, experimental research of interfacial properties has always been a difficult and challenging task. Beside the experimental techniques, molecular dynamics (MD) simulations can be used to get new insights into the topic of wetting phenomena.

In the last decade, MD simulations have been used to understand different properties of pure liquids, mixture of different liquids and also liquid interfaces. With the development of molecular simulation techniques, it is possible to obtain information at the molecular scale like the orientation of molecules where the solid, liquid and gas phases meet. Such

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information is impossible or hard to obtain from experiments. In defining the wetting characteristics of a solid surface by a liquid, there are several interaction terms (like the solid-liquid and the liquid-liquid interactions) that are contributing. The contribution of different terms, however, cannot be separated in experiments. Changing one of these parameters will lead to change some other parameters.

Outlook

MD simulations can be used as a tools to investigate the effect of different parameters separately. The behavior of a liquid near a surface depends upon the strength and the range of the intermolecular (liquid-liquid and liquid-substrate) interactions and on the structural properties of the substrate. The main goal of this project is to understand the wetting behavior of a system in terms of the molecular interactions, and indentify the contribution of different interactions to the wetting properties by using the computer simulation.

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