Using molecular simulation to understand wetting at rough surfaces

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Fluids routinely interact with solid substrates in industrial processes, natural phenomena, and throughout our daily experiences. Examples vary from the use of liquid detergents to clean stained fabric to the collection of rain water onto tree leaves. The behavior of a fluid in the vicinity of a surface depends qualitatively upon the relative strengths and ranges of the fluid-fluid and fluid-substrate interactions and the structural characteristics of the substrate. It is the latter of these factors that we focus on here. In this presentation, we describe our recent efforts aimed towards obtaining a better understanding of the effect of surface roughness on wetting behavior through the use of molecular simulation. We will first focus on the anisotropic nature of wetting at crystalline solids, which is related to the distinct spreading properties a fluid displays when placed in contact with different crystalline faces (e.g. 100, 110, 111). We will then examine the effect of nanoscale surface roughness (substrates with hills and valleys that have heights and widths in the 1-10 nm range) on wetting behavior. More specifically, we will examine the evolution of the contact angle with variation of the amplitude and length scale of geometric heterogeneities. Our simulation-based results will be compared with macroscopically-based expressions for describing the influence of roughness, such as those due to Wenzel and Cassie.

FRIDAY, March 13, 2009
2:00 – 3:00 p.m.
BOGGS ROOM 243

Refreshments will be served before the seminar.