269d Molecular Models of Wetting of Porous Solid Surfaces: Understanding Superhydrophobicity

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Understanding the wetting of corrugated and porous surfaces by liquids is a problem of long standing interest in areas ranging from textile science to catalytic reaction engineering. Renewed interest in this problem has been generated by discoveries of surfaces with small scale corrugations that exhibit very large contact angles for water or other liquids - in some cases the contact angles are close to 180 degrees. Such surfaces are referred to as superhydrophic or ultrahydrophic. In this work we investigate the extent to which these systems can be described using statistical mechanics. We consider the case where the solid surface is covered with an array of uniformly spaced pillars and we describe the system using a lattice fluid model. This model can be treated using mean field density functional theory from which we can calculate the three-dimensional density distribution for liquid drops on corrugated surfaces. We find that the behavior seen in the recent experiments can indeed be described in this way. The use of a lattice model allows us to bridge the molecular and mesoscopic length scales. We use our approach to investigate the accuracy of classical approaches to estimating contact angles for these systems including the Wenzel and Cassie-Baxter equations.