

Abstract Submitted  
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**Spreading of a Nanodroplet on a Solid Surface Physically-Patterned with an Array of Pillars**<sup>1</sup> HONGFEI WU, KRISTEN FICHTHORN, ALI BORHAN, Chemical Engineering Department, The Pennsylvania State University — Molecular dynamics simulations are used to study the spreading dynamics of a Lennard-Jones liquid droplet on a heterogeneous solid surface. The solid is physically patterned by placing a set of pillars of square or circular cross section on an otherwise flat surface. The liquid-solid interaction is modeled by a modified Steele's potential derived for arrays of pillars characterized by a desired roughness and solid fraction. Using the modified Steele's potential, liquid-solid interactions can be computed more quickly, and larger droplet sizes can be studied. Simulations indicate that the spreading of nanodroplets depends not only on the surface energy of the solid, but also on the heterogeneity of the solid surface. For a constant solid surface energy, the topographic structure of the solid surface can have a significant effect on its hydrophobic characteristics. By varying the pillar height, spacing, and arrangement on the solid surface, a transition between the Wenzel and Cassie modes of wetting is observed in the simulations. These observations are explored in terms of the interplay between the bulk liquid chemical potential and the liquid-solid interfacial tension, as well as the topology of the liquid-solid potential-energy surface induced by surface heterogeneity.

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Hongfei Wu  
Chemical Engineering Department, The Pennsylvania State University

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