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Theory and Simulation of Droplet Wetting on Patterned Surfaces<sup>1</sup> AZAR SHAHRAZ, ALI BORHAN, KRISTEN FICHTHORN, Penn State University — Liquid droplets can have multiple wetting modes on physically patterned surfaces, each corresponding to a (meta)stable state. For example, in the Cassie mode, the droplet resides on top of the pattern, while in the Wenzel mode, the droplet penetrates into the pattern. In this work, we study the wetting of patterned surfaces on two different length scales: on the nano-scale using molecular dynamics (MD) and on the macro-scale by minimizing free-energy expressions for various droplet wetting modes. We find that surface topography, size, and initial position of the droplet strongly affect the wetting states and contact angles. In the small Bond-number (small droplet) regime, the surface topography can be scaled by the droplet size, such that the preferred wetting modes and contact angles become independent of droplet size for surfaces with the same scaled topography. MD simulations and theory are in good agreement for small Bond numbers. For moderate to large Bond numbers, gravity plays an important role and MD simulations cannot accurately describe wetting. We create wetting phase diagrams and find that our predictions are in good agreement with experiment. The resulting wetting phase diagrams may serve as a guideline in creating surfaces with desired wettability.

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