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Use of the string method to find minimal energy paths of droplets on superhydrophobic surfaces KELLEN PETERSEN, Courant Institute of Mathematical Science, New York University — Interest in superhydrophobic surfaces has increased due to interesting advances in science and engineering. Here we use a diffuse interface model for droplets on topographically and chemically patterned surfaces. We then apply the constrained string method to examine the transition of droplets between different metastable/stable states. The string method finds the minimal energy paths (MEPs) which correspond to the most probable transition pathways between the metastable/stable states in the configuration space. In the case of a hydrophobic surface we determine the MEP corresponding to the transition between the Cassie-Baxter and Wenzel states. Additionally, we realize critical droplet morphologies along the MEP associated with saddle points of the free-energy potential and the energy barrier of the free energy. We analyze and compare the MEPs and free-energy barriers for a variety of surface geometries, droplets sizes, and static contact angles ranging. We demonstrate the string method as a useful tool in the study of droplets on superhydrophobic surfaces by presenting a numerical study that finds MEPs in configuration space, critical droplet morphologies and free-energy barriers which in turn give us a greater understanding of the free-energy landscape.

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