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Numerical study of wetting transition on patterned hydrophobic surfaces using the string method WEIQING REN, National University of Singapore and IHPC — We study the wetting transition on micro-structured hydrophobic surfaces using the string method. On a patterned solid surface, a liquid droplet can exhibit the suspended Cassie-Baxter state, or impaled Wenzel state. We compute the transition states, the energy barriers, and the minimum energy paths for the wetting transition from the Cassie-Baxter state to the Wenzel state. Numerical results are obtained for the wetting of a hydrophobic surface textured with a square lattice of pillars. It is found that the wetting of the solid substrate occurs via infiltration of the liquid in a single groove, followed by lateral propagation of the liquid front. The propagation of the liquid front proceeds in a stepwise manner, and a zipping mechanism is observed during the infiltration of each layer. The minimum energy path for the wetting transition goes through a sequence of intermediate metastable states, whose wetted areas reflect the micro structure of the patterned surface.

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