

Abstract Submitted  
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**Validation of Capillarity Theory at the Nanometer Scale by Atomistic Computer Simulations of Water Droplets and Bridges in Contact with Hydrophobic and Hydrophilic Surfaces** NICOLAS GIOVAMBATTISTA, CUNY-Brooklyn Coll, ALEXANDRE ALMEIDA, ADRIANO ALENKAR, Instituto de Física, Universidade de São Paulo, 05508-090, São Paulo, SP, Brazil, SERGEY BULDYREV, Department of Physics, Yeshiva University, 500 West 185th Street, New York, New York 10033, United States — Capillarity is the study of interfaces between two immiscible liquids or between a liquid and a vapor. Capillarity theory (CT) was created in the early 1800s and it is applicable to macroscopic ( $>1 \mu\text{m}$ ) systems. In general, macroscopic theories are expected to fail at  $<10 \text{ nm}$  scales where molecular details may become relevant. We show that, surprisingly, CT provides satisfactory predictions at 210 nm scales. Specifically, we perform atomistic molecular dynamics (MD) simulations of water droplets and capillary bridges of different symmetry in contact with various surfaces. The surfaces correspond to hydroxylated silica, modified to cover a wide range of hydrophobicity/hydrophilicity. In agreement with CT, it is found that (i) water contact angle is independent of the droplet/bridge geometry and depends only on the surface employed; (ii) CT provides the correct droplet/bridge profile for all hydrophobic/hydrophilic surfaces considered; and, remarkably, (iii) CT works even for the very small droplets/bridges studied, for which the smallest dimension is  $\approx 2 \text{ nm}$ . We confirm the self-consistency of CT at 210 nm scales by calculating the *capillary forces* between different surfaces induced by capillary bridges; the agreement between MD simulations and CT theory is remarkable

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