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Hydration and Dewetting near Fluorinated Superhydrophobic Plates RUHONG ZHOU, XIN LI, JINGYUAN LI, MARIA ELEFTHERIOU — The water dynamics near a nanoscale fluorinated ($CF_3(CF_2)_7(CH_2)_2SiH_3$) surface as well as the possible dewetting (water drying) transition within two such superhydrophobic surfaces (plates) have been studied with molecular dynamics simulations. A partial water dewetting with an expansion of approximately 7-8Å and a water density ∼20% lower than the bulk is found near the single superhydrophobic surface. More remarkably, a strong dewetting transition is found in the inter-plate region for the double plates with a critical distance D_c up to 10Å (3-4 water diameters). This transition, although occurring on a microscopic length scale, is reminiscent of a first order phase transition from liquid to vapor. Furthermore, simulation results show that the fluorinated carbons are more hydrophobic than their hydrogenated counterparts (with $D_c = 8.0$Å) in terms of the dewetting transition critical distance, despite their much larger partial charges and dipoles. The unusual superhydrophobicity of fluorocarbons is found to be related to their larger surface areas, while the intrinsic hydrophobicity is roughly the same for both fluorocarbons and hydrocarbons based on a detailed water-plate interaction energy profiling. Somewhat surprisingly, we find that even though the electrostatic energies do contribute slightly more in the fluorocarbon plates than the hydrocarbon plates, the van der Waals energies dominate the water-plate interactions (with more than 90% contributions for close shells) and they contribute almost the same in both plates.

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