Fluctuations of Water near Hydrophobic, Hydrophilic and Patterned Surfaces and in Nanoscopic Confinement

AMISH PATEL, DAVID CHANDLER, University of California, Berkeley, SUMANTH JAMADAGNI, HARI ACHARYA, SHEKHAR GARDE, Rensselaer Polytechnic Institute — We study water density fluctuations in probe volumes of different shapes and sizes, in the bulk, near various hydrophobic and hydrophilic surfaces as well as in nanoscopic confinement between these surfaces. Specifically, we report the probability of finding $N$ water molecules in large ($>1 \text{ nm}^3$) probe volumes. An examination of these large length-scale fluctuations of water near a hydrophobic surface reveals that the probability of density depletion is significantly larger than that in bulk, akin to density fluctuations near a water-vapor interface. In contrast, fluctuations near a hydrophilic surface are very similar to that in the bulk. We further investigate the effect of surface heterogeneity on fluctuations. We also examine the effect of confinement on density fluctuations as a function of the nature of the confining surfaces as well as the distance between them.

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