73d Computational Study of Structure and Dynamics of Water near Surfaces with Controlled Hydrophobicity

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We present a numerical investigation of water structure and dynamics near nanoscale surfaces with tunable hydrophobicity. The system we consider consists of some 3000 SPC/E water molecules and two parallel plates of hydroxylated silica (ca 800 atoms each). We control hydrophobicity by varying the composition and charge distribution of the walls. We investigate the effects of pressure (2 kbars to -1kbar), wall separation, and spatial distribution of hydrophobicity upon water structure and dynamics, with particular attention paid to dewetting phenomena. We find that the specific manner in which a given fraction of hydrophobic sites is distributed on the surface has a profound effect on water structure and dynamics. The dewetting phenomenology is also found to be sensitively dependent upon applied pressure.