Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Influence of dissolved gasses on hydrophobic interaction at different length-scales[1] ALENKA LUZAR, Department of Chemistry, Virginia Commonwealth University (VCU), 1001 West Main Street, Richmond, VA 23284-2006, D. BRATKO[2], University of California at Berkeley — Despite widespread experimental evidence of the influence of dissolved gases on hydrophobic interaction, the mechanism of observed effects are still unknown. We present direct calculations of the hydrophobic force between model hydrophobic surfaces in the presence and absence of dissolved gases, and varying surface separation up to 4 nm. We monitor gas adsorption at molecular resolution inaccessible to experiments. We find insignificant gas adsorption, confined to the first molecular layer, and no dependence of the width of the perturbed water layer on the amount and type of dissolved gas. The results offer a molecular-level interpretation for the lack of influence of dissolved gas on the short-range hydrophobic force, a finding that is consistently reported in experiments that show a dramatic gas effect at long-range, but minimal at short-range or in determining the adhesion force or interfacial energy. Finally, a coarse-grained approach is discussed to deal with apparent non-equilibrium effects at longer-range and implications to biological systems and nanoscience.

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Date submitted: 02 Dec 2007 Electronic form version 1.4