

Abstract Submitted
for the DFD05 Meeting of
The American Physical Society

Liquid-Gas Mixtures in Contact with Walls: Molecular Simulations STEPHAN MARKUS DAMMER, DETLEF LOHSE, Physics of Fluids, University of Twente — We perform molecular dynamics simulations of liquid-gas mixtures in contact to solid walls. We present results concerning Lennard-Jones systems composed of three particle species, namely liquid, foreign gas, and wall particles, which are frozen on a lattice: (i) Close to the wall we observe a layering of the fluid which becomes more pronounced for increasingly hydrophilic walls. (ii) Close to smooth hydrophobic walls we find a two orders of magnitude increase in the number density of gas, which will favor bubble nucleation. (iii) To characterize the walls, we determined the contact angle by simulations of droplets and compare the result to Laplace's estimate of surface energies.

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Date submitted: 09 Aug 2005

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