Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Computational investigation of wetting and prewetting phase behavior[1] JEFFREY ERRINGTON, Dept. of Chemical and Biological Engineering, University at Buffalo — Fluids in the presence of one or more surfaces exhibit a rich variety of phase transitions that are absent in bulk fluids. Even the simplest of systems display a broad range of phase behavior. In this presentation, we describe our recent efforts aimed towards obtaining a better understanding of surface phase behavior through the use of molecular simulation. The first part of the presentation will be used to provide an overview of transition-matrix based Monte Carlo algorithms that enable one to efficiently locate and characterize phase transitions. Results will then be presented that describe how the wetting behavior of a model substrate-fluid system evolves with temperature and the relative strength of the substrate-fluid interaction. Simulation results will be compared with density functional theory calculations. Finally, we will describe a series of calculations that enable us to estimate the boundary tension along the prewetting saturation line. This quantity is related to the line tension associated with the formation of liquid droplets on a solid substrate. The magnitude of this tension has been the subject of debate recently, with experimental values spanning several orders of magnitude.

[1]This material is based upon work supported by the National Science Foundation under Grant No. CTS-0238772.

Jeffrey Errington
Dept. of Chemical and Biological Engineering, University at Buffalo

Date submitted: 30 Nov 2005 Electronic form version 1.4