Fluid Phase Equilibria for SSSW Potentials Predicted Using Monte Carlo Simulations in the Gibbs Ensemble JOHN WHITE, American University — Monte Carlo free energy calculations have been undertaken using the Gibbs ensemble method[1] for a fluid of hard spheres with repulsive square shoulders next to attractive square wells in order to predict properties of the fluid both above and below the gas-liquid critical point. In addition, for some choices of square-shoulder height and width and square-well depth and width there is at a lower temperature a transition to two-phase high density and low density liquid. Results will be presented and compared with published results of some molecular dynamics simulations and discussed in relation to the conjectured liquid- liquid phase transition in water.

[1]See A. Z. Panagiotopoulos, Mol. Sim. 9:1-23, 1992, and Ch. 8 in D. Frenkel and B. Smit. Understanding Molecular Simulation From Algorithms to Applications. Academic Press, Elsevier, London, 2002.

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