Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A SAFT-based classical density functional for water DAVID ROUNDY, JESSICA HUGHES, ERIC KREBS, Oregon State University — We present a new classical density functional for water based on a combination of Statistical Associating Fluid Theory (SAFT-VR) with the Fundamental Measure Theory (FMT) functional for the hard-sphere fluid. In the homogeneous limit, our functional reduces to the the published optimal SAFT model of Clark *et al* [1]. By adding a single fitting parameter, we reproduce the bulk surface tension of water within a wide temperature range. We will present results for hydrophobic hard rods and spheres, including the temperature dependence of the hydrophobic interaction.

[1] G. Clak, A. Haslam, A. Galindo, and G. Jackson, Molecular Physics **104**, 3561 (2006).

David Roundy
Oregon State University

Date submitted: 12 Dec 2011 Electronic form version 1.4