Abstract Submitted for the NWS08 Meeting of The American Physical Society

Hydrophobic Interactions in Multiple Scales Using Density-Functional Theory DENNIS JACKSON, Oregon State University, DAVID ROUNDY, Oregon State University — We present a classical density functional for water that represents the short-range repulsive interaction using a fundamentalmeasure-theory (FMT) hard-sphere functional, in addition to a functional that represents the attractive interaction between molecules. The parameters of these functionals are chosen to reproduce the experimental liquid density, bulk modulus and surface tension of water, and to ensure coexistance of liquid and vapor phases. The functional inherits from the FMT functional its accurate description of reduceddimensionality configurations. We will present computations of the hydrophobic hydration energy of hard-sphere solutes, demonstrating an accurate description at both large and small length scales.

> Dennis Jackson Oregon State University

Date submitted: 15 Apr 2008

Electronic form version 1.4