

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

A classical density functional for water DAVID ROUNDY, DENNIS JACKSON, Oregon State University — We present a classical density functional for water that represents the short-range repulsive interaction using the fundamental-measure-theory hard-sphere functional. The parameters of this functional are chosen to reproduce the experimental liquid density, bulk modulus and surface tension of water, and to ensure coexistence of liquid and vapor phases. This functional inherits from the FMT functional its accurate description of reduced-dimensionality 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.

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Date submitted: 27 Nov 2007

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