

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Incorporation of an Improved Radial Distribution Function into Classical DFT JOOST DE GUSSEM, ERIN MCGARRITY, Delft Technical University — An expression for the radial distribution function $g(\vec{r})$ for a fluid can be found using classical density functional theory. We use this expression in place of the mean-field value (*e.g.*, $g = 1$ for Lennard Jones fluids) in the excess Helmholtz free energy functional for the pair interactions to achieve self-consistent density profiles. We will discuss the differences found with this improved choice for $g(\vec{r})$ compared to other, simpler approximations. We will show results for liquid-vapor systems containing hard-sphere fluids with Lennard-Jones and dipolar interactions.

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Date submitted: 11 Nov 2011

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