2003 Vol.39 No.2 pp.231-237 DOI:

A New Uniform Phase Bridge Functional: Test and Its Application to Non-uniform Phase Fluid

ZHOU Shi-Qi, CHEN Hong, and ZHANG Xiao-Qi

Research Institute of Modern Statistical Mechanics, Zhuzhou Institute of Technology, Zhuzhou 412008, China
(Received: 2002-4-15; Revised: 2002-7-2)

Abstract: A new bridge functional as a function of indirect correlation function was proposed, which was based on analysis on the asymptotic behavior of the Ornstein-Zernike (OZ) equation system and a series expansion whose renormalization resulted in an adjustable parameter determined by the thermodynamics consistency condition. The proposed bridge functional was tested by applying it to bulk hard sphere and hard core Yukawa fluid for the prediction of structure and thermodynamics properties based on the OZ equation. As an application, the present bridge functional was employed for non-uniform fluid of the above two kinds by means of the density functional theory methodology, the resulting density distribution profiles were in good agreement with the available computer simulation data.

PACS: 61.20.Gy
Key words: bridge functional, density functional theory, direct correlation function

[Full text: PDF]

Close