

Quantitative Description of Potential of Mean Force Between Macroparticles in Fluid with Attractive Forces

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Abstract: A statistical mechanics method is proposed for calculation of potential of mean force (PMF). In the case of solvophobic or solvophilic macroparticles immersed in solvent bath of soft sphere or Lennard-Jones particles, prediction accuracy for the PMF and MF from the simplest implementation of the proposed method, where hypernetted chain approximation is adopted for correlation of the macroparticle-macroparticle at infinitely dilute limit, is comparable to that of a recent more sophisticated approach based on mixture Ornstein-Zernike integral equation / bridge function from fundamental measure functional. Adaptation of the present method for general complex fluids is discussed, and method for improving the accuracy is suggested. Differences and relative merits of the present recipe compared with that based on potential distribution theory is discussed.

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Key words: potential of mean force, colloid, density functional theory

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