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Accuracy of Solvation Free Energy Estimated from Integral Equation Theory for Two-Component System of Lennard-Jones Fluid TATSUHIKO MIYATA, JYOTI THAPA, Department of Physics, Ehime University — Solvation of complex molecules has attracted many researchers. Typically they employ molecular dynamics (MD) simulations to calculate solvation free energy (SFE), whereas there is another route to calculate SFE: i.e., integral equation theory (IET). One of the IETs to calculate SFE for molecular liquid is three-dimensional reference interaction site model (3D-RISM) theory. 3D-RISM can calculate SFE with cheaper computer cost than MD, which is one of the advantages of the theory. Though 3D-RISM significantly improved the description of solvation in comparison with a traditional IET, the accuracy of SFE evaluated from the theory was still unsatisfactory. Our final goal is to develop a new theoretical tool to calculate SFE with satisfactory accuracy and relatively cheap computer cost. As a first step, this study examines how IET is accurate or inaccurate in terms of SFE. For simplicity, we choose Lennard-Jones systems composed of two components (i.e. solute and solvent). In particular, we focus on two approximations used in IET, i.e., hypernetted chain and Kovalenko-Hirata approximations We discuss the accuracy of these approximations by comparing SFEs evaluated from the corresponding approximations with those from MD simulations.

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