CC-RISM Theory

Kanchana S. Thanthiriwatte and Steven R. Gwaltney

Department of Chemistry, Center for Environmental Health Sciences, and HPC^2 Center for Computational Sciences, Mississippi State University Mississippi State, MS 39762, USA.

Abstract

We report the theory for and the implementation of the reference interaction site model (RISM) for solute-solvent systems at the coupled-cluster singles and doubles (CCSD) level. The idea of the method is to replace the reaction field in continuum models by a microscopic expression in terms of the site-site radial distribution functions between solute and solvent, which can be calculated from the RISM integral equations. The statistical solvent distribution around the solute is determined based on the electronic structure of the solute, while the electronic structure of solute is influenced by the surrounding solvent distribution. Therefore the orbitals and the RISM equations are solved self-consistently with CCSD. To evaluate the accuracy of the present method, test calculations have been carried out for a number of small molecules.