

Coupling QC, MTS-MD, And DPD With Molecular Theory Of Solvation In A Framework Of Multiscale Methods

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Abstract

Multiscale modeling has been energetically developing in recent decades. Multiscale approximations are popular in theoretical developments, as they dramatically improve accuracy, efficiency, and applicability by self-consistently coupling models and methods at different length and time scales. This work reviews and addresses the combination of quantum chemistry methods, molecular theory of solvation, multiple time step molecular dynamics, and dissipative particle dynamics simulations in modern material and biomolecular science. The novel approach provides fundamental understanding and predictions in a number of areas of research and applications. This also leads to a special role in commercialization by quickly evaluating new research projects and guiding new developments. A central role in this framework of multiscale modeling is given to molecular theory of solvation which accurately introduces the effect of environment on complex nanomolecular and biomolecular system. The approach can be naturally coupled with full range of computational chemistry approaches, including quantum mechanics, molecular mechanics, coarse grained methods in dissipative particle dynamics, and the variety of COMSOL multiphysics approaches. Illustrative examples here include analytical differentiation of the free energy functionals and self-consistent coupling of the statistical-mechanical, three-dimensional reference interaction site model with Kovalenko-Hirata closure relation (3D-RISM-KH) molecular theory of solvation with the KS-DFT and CASSCF quantum chemistry methods in a self-consistent field description of electronic structure, geometry optimization, nanochemistry, and photochemistry in solution. Multiple time step molecular dynamics of biomolecules steered by effective solvation forces obtained from the 3D-RISM-KH theory is accelerated by the generalized solvation force extrapolation (GSFE) and stabilized by the optimized isokinetic Nosé-Hoover chain (OIN) thermostat. This enables gigantic outer time steps up to tens picoseconds to accurately calculate equilibrium properties. The method thus constitutes a framework of multiscale quasidynamics, a new essential approach to very slow dynamics of compounds, biomolecules, and nanostructures in modern areas of nanoscience and nanotechnology.

Keywords: Solvation, 3D-RISM-KH, KS-DFT, multiple time step MD, generalized solvation force extrapolation, molecular mechanics, DPD, coarse graining