What's New in Q-Chem

Smooth Polarizable Continuum Implicit Solvent Models

Developers: Adrian W. Lange and John M. Herbert

Solvent effects play an important role in many quantum chemistry applications, and polarizable continuum models (PCMs) provide a simple and efficient means to incorporate bulk solvent effects. We have implemented PCMs with a special numerical integration method, called the switching/Gaussian (SWIG) method that ensures continuity and smoothness of the solute's potential energy surface, despite the finite-element nature of PCMs. Our implementation is therefore stable for applications such as geometry optimizations and *ab initio* molecular dynamics simulations, where continuous forces are required. It is also available for MM/PCM and QM/MM/PCM calculations. PCMs can model electrostatic interactions with a solvent, given the solvent's bulk dielectric constant. For example, room temperature water can be modeled as a structureless dielectric medium with ε=78.

We have also implemented a number of features that make PCM calculations scale linearly (in both CPU time and memory) with respect to system size. This facilitates MM/PCM and QM/MM/PCM calculations with large MM regions.

John Herbert

Adrian Lange

Publications:

A.W. Lange and J.M. Herbert, "Polarizable Continuum Reaction-Field Solvation Models Affording Smooth Potential Energy Surfaces" *J. Phys. Chem. Lett.* **1**, 556 (2010)

A.W. Lange and J.M. Herbert, "A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: The switching/ Gaussian approach" *J. Chem. Phys.* **133**, 244111 (2010)

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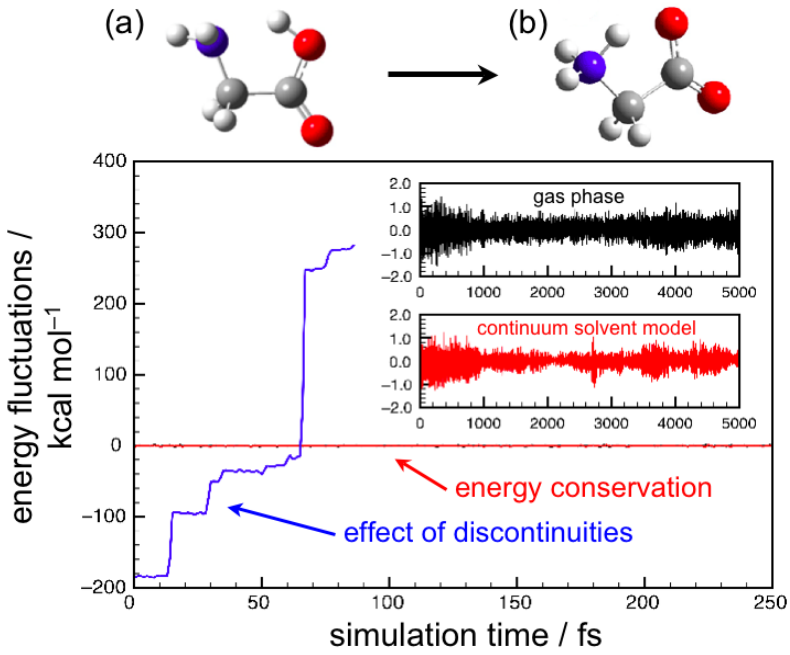
What's New in Q-Chem

Smooth Polarizable Continuum Implicit Solvent Models (continued)



Energy fluctuations during an *ab initio* molecular dynamics simulations of glycine (described at teh PBE0/6-31+G* level) in water (modeled using a PCM with $\varepsilon = 78$). Starting from the gas-phase amino-carboxy tautomer (a), the molecule undergoes a spontaneous intramolecular proton transfer to form the zwitterionic tautomer (b). Using our SWIG implementation of the solvent model, the solution-phase simulation (energy fluctuations shown in red) is as stable as a gas-phase simulation (energy fluctuations shown in black), despite the proton-transfer event, which dramatically alters the shape of the solute cavity. A more straightforward discretization of the PCM equations (energy fluctuations in blue) leads to instabilities that ultimately cause the simulation to fail.

For more information on how to use this feature, refer to the Q-Chem Manual, Section 10.2.2-10.2.4.

For more new features, visit:
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