A Polarizable Continuum Model of solvation designed for QMC: ground and excited states of solutes.

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We show a novel Polarizable Continuum Model (PCM) scheme we have developed to include both surface and volume polarization of the dielectric medium. In particular, the treatment of volume polarization, due to quantum mechanical penetration of the solute charge density in the solvent domain, is based on quantum Monte Carlo techniques. The method allows to accurately solve Poisson's equation of the solvation model coupled with the Schrödinger equation for the solute [1,2]. The performance of the approach has been verified on a representative set of solutes in water as solvent [2] and in the transfer of glutamic acid and related ions from a lipidic phase to water [3]. The present model has been recently extended to treat the effects of solvation in solute vertical electronic transitions. Some results on $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ vertical transition of *s*-trans-acrolein in water are here presented [4].

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