THE SWITCHING/GAUSSIAN METHOD FOR POLARIZABLE CONTINUUM MODELS WITH APPLICATIONS TO AQUEOUS MOLECULAR DYNAMICS AND VIBRATIONAL SPECTRA

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We describe the recently-developed Switching/Gaussian (SWIG) formalism for polarizable continuum models (PCMs) in electronic structure theory and QM/MM calculations. Existing PCM implementations are well-established, yet still exhibit Coulomb singularities and/or discontinuities in potential energy surfaces, which result from the finite-element discretization of the solute–continuum interface. Our revised implementation eliminates these problems. We illustrate the robustness this approach using *ab initio* molecular dynamics and vibrational spectra calculations, for which existing PCM implementations fail. Furthermore, we present the extension of SWIG to unprecedentedly large systems, making it a viable implicit solvation method even for molecular mechanics calculations of biological macromolecules.