EXCITED STATES IN SOLUTION AT EOM-CCSD LEVEL WITH THE POLARIZABLE CONTINUUM MODEL OF SOLVATION

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Electronic excited states are at the center of many research areas, and theoretical simulations are increasingly important. Although approximate methods based on time dependent density functional theory represent a useful tool, accurate wave function methods are still the most reliable approach. These methods, however, suffer from high computational cost that limits their range of applicability. This is particularly so when the system under study is in solution. In fact, the treatment of a large number of solvent molecules, even when modeled at a low level of theory (like molecular mechanics), is cumbersome due to the large number of conformations that needs to be considered. When the solvent is not directly involved in the process, its effect can be properly accounted for by using polarizable continuum models (PCMs) where the conformational average is implicit in the solvent dielectric constant. In this contribution, the treatment of electronic excited state energy and structure of molecules in solution at the EOM-CCSD/PCM level of theory is presented. This approach represents an effective compromise between computational cost and accurate treatment of the central part of the system while taking into account the non-negligible effect of the solvent.