Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach

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We present a new implementation of continuum solvation models for semiempirical Hamiltonians that allows the description of environmental effects on very large molecular systems. In this approach based on a domain decomposition strategy of the COSMO model (ddCOSMO), the solution to the COSMO equations is no longer the computational bottleneck but becomes a negligible part of the overall computation time. In this Letter, we analyze the computational impact of COSMO on the solution of the SCF equations for large to very large molecules, using semiempirical Hamiltonians, for both the new ddCOSMO implementation and the most recent, linear scaling one, based on the fast multipole method. A further analysis is on the simulation of the UV/visible spectrum of a light-harvesting pigment–protein complex. All of the results show how the new ddCOSMO algorithm paves the way to routine computations for large molecular systems in the condensed phase.

This is a joint work with
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