

# Molecular properties in solution

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Solvent effects are of essential importance in many different aspects of physics, chemistry, biology and material sciences. The developments of quantum chemistry methods originally devised for studying isolated molecules have been extended to study the properties of atoms and molecules interacting with the environment. This led to the continuum methods that treat the solvent by means of average macroscopic constants, such as the dielectric constants. Very successful in different applications these continuum methods lack the consideration of the microscopic details and the necessary statistic representation of the liquid system. The natural extension has been to incorporate some computer simulation method to represent the structures of the liquid and couple this with the necessary quantum mechanical method, necessary to obtain spectroscopic and structural properties. This is the essence of the so-called QM/MM methods where part of the system is treated by molecular mechanics whereas the remaining is treated by quantum mechanics. We have been involved in the developments of a sequential procedure (S-QM/MM) where the computer simulation is used to obtain the structures of the liquid for subsequent QM calculations. The advantage over the conventional QM/MM methodology is that by a simple and proper sampling statistically converged properties can be assured. The disadvantage is that the QM and the MM parts need special care in the coupling procedure. In this presentation we report on the new developments of this methodology and we address to solvatochromic shifts and in special the spectroscopic properties of ortho-betaine in water.

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