Theoretical Studies of Solvent Effects in Electronic Properties of Molecules with Biophysical Interest

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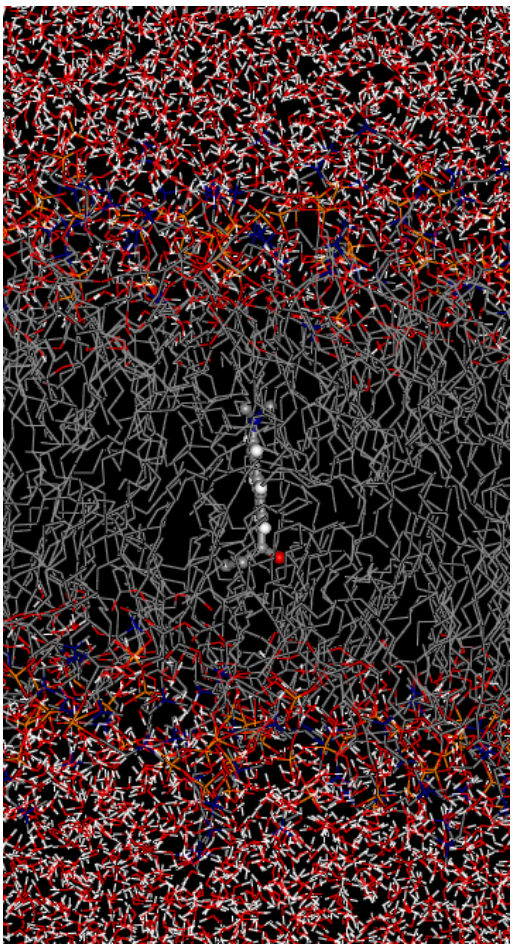

Solvent effects are of essential importance in many different aspects of physics, chemistry, biology and material sciences. The developments of quantum chemistry methods originally devised for studying isolated molecules have been extended to study the properties of atoms and molecules interacting with 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 thermodynamic molecular system. The natural extension has been to incorporate some molecular mechanic methods to generate solute-solvent structures and couple this with the quantum mechanical methods to obtain the solvent effects in the solute properties. This is the essence of the so-called QM/MM methods where part of the system is treated by molecular mechanics (MM) whereas the remaining is treated by quantum mechanics (QM). We have been involved in the developments of a sequential procedure (S-QM/MM)[1] where the MM simulations are used to obtain the structures of the solution for subsequent QM calculations. In this presentation we report some developments [2,3] of this methodology and we address to some applications in electronic polarization and spectrum [4-7] for some organic molecules in different environments, such as homogeneous liquid, mixtures and phospholipid membranes.

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