Theoretical Studies of Electronic Structure of Molecules Interacting with Phospholipid Bilayers

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Molecular surrounding or solvent effects are of essential importance in many different aspects of physics, chemistry, biology and material sciences. The developments of Quantum Mechanics methods devised for studying electronic and structural properties of isolated molecules have been extended to study the properties of molecules in solution. This led to the Continuum Models 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, the heterogeneous description of more complex molecular surroundings such as lipid membranes and the necessary statistic representation of the thermodynamic molecular system. The natural extension has been to incorporate Molecular Mechanics methods to generate solute-solvent configurations and couple this with the quantum mechanical methods to obtain the solvent effects in the solute properties. We have been involved in the developments and applications of such methodologies. In this presentation we report some developments and address to some applications in polarization and electronic spectra for some organic molecules in different environments: solution [1,2] and phospholipidic bilayers [3,4].

References

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