Simulation of Molecular Spectroscopy in Complex Environments

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Effects of the interaction of a reference molecule with an environment are of essential importance for the understanding of many different aspects of physics, chemistry, biology and material sciences. The developments of quantum mechanics originally devised for studying isolated molecules have been extended to study the properties of atoms and molecules interacting with a liquid system or a more complex environment. Successful in different applications the use of dielectric-type or continuum methods lack the consideration of the microscopic details and the necessary statistical representation of real liquid systems. The natural extension has been to incorporate statistical mechanics to represent the structures of the liquid and couple this with the necessary quantum mechanical method, to obtain spectroscopic and structural properties. To ensure statistically converged results this is done sequentially. Monte Carlo or Molecular Dynamics simulation generates structure for subsequent QM calculations. In this work we report some applications of this S-QM/MM in different parts of the phase diagram, thus considering both liquid and supercritical environments. To proceed further we have developed a procedure for obtaining free energy gradient thus incorporating relaxation in the environment. Application will consider the absorption spectrum of rhodopsin in the complex environment of a protein.

This work has been supported by CNPq, CAPES and FAPESP (Brazil)