

Environment Contribution to Molecular Spectroscopy, Reactivity and Photochemistry.

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The combination of quantum mechanics (QM) with molecular modeling (MM) is a powerful tool for studies of simple and complex liquids. In addition, it may also be used to study the spectroscopic and reactivity of molecules in solution, a situation that is germane in chemical laboratories. The understanding of the solvent effects is thus a major concern in the rationalization of experimental results. In the last two decades theoretical treatments have been developed to incorporate solvent effects. An important direction of research uses some sort of computer simulation to perform hybrid calculations. This is generally called QM/MM method, because both classical and quantum methodologies are employed. In fact the simulations can be performed both at the classical (e.g. Monte Carlo or Molecular Dynamics) or quantum levels (e.g. Born-Oppenheimer Molecular Dynamics). As long as the thermodynamic condition can be imposed this opens a large avenue for applications in other parts of the phase diagram. Hence, it is also possible to address the technologically and environmental friendly condition of supercritical fluids. A simple protocol where the quantum mechanics calculations are performed subsequent on structures generated by the liquid simulations has been developed along the past years and guarantees efficiency and statistical convergence of the results [1]. Different applications have been made in spectroscopy and reactivity both in regular liquid environment as well as in supercritical condition. A critical review of this sequential QM/MM using either Monte Carlo or Born-Oppenheimer Molecular Dynamics will be presented based on a large variety of applications [2-10] on absorption and emission spectroscopy, magnetic shielding related to NMR experiments, excited state dynamics of simple organic molecules, simple chemical reactions as well as some photophysical processes. Some perspectives will also be presented.

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