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Abstract: Solvent effects are of essential importance in many different aspects of physics, chemistry, biology and material sciences [1]. 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 [2,3] 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 mechanics 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) [4,5]. …….

Key-words: ……..
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