Properties and Spectroscopy of Molecules in Simple and Complex Environments. An efficient Implementation of the Sequential QM/MM with Free Energy Gradient.

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Combining quantum mechanics (QM) with classical molecular modeling (MM) leads to a powerful tool for studies of non-isolated molecules. This hybrid and multiscale method allows studying molecules in simple and complex environments. This is generally called QM/MM method and it may be used to study the properties, spectroscopy and reactivity of molecules in solution, as well as molecules in more complex environments such as critical fluids, proteins and even the vicinities of a critical point. A simple review will be presented of our methodology to calculate free energy (and free energy gradients) of molecules in solution using the average solvent electrostatic configuration in combination with a van der Waals embedding. The sequential QM/MM ASEC-vdW-FEG, using either Monte Carlo or Molecular Dynamics has been implemented and a variety of applications of molecular properties and spectroscopy will be shown in different environments, such as simple homogeneous liquids, supercritical fluids and proteins [1].

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References: see http://portal.if.usp.br/gfmm/canuto