Reunião Anual do INCT-FCx - 2022

De 26 a 29/Outubro de 2022,
Hotel Estância Atibainha, Nazaré Paulista/SP

Simulation of Molecular Spectroscopy in Simple and Complex Environments

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Abstract: 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 of the methodology developed in our laboratory, the sequential QM/MM, using either Monte Carlo or Molecular Dynamics will be presented 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.

Key-words: Molecular spectroscopy, complex environment, QM/MM.

Support: This work has been supported by CNPq, CAPES, FAPESP and INCT FCx