FULLY ATOMISTIC EMBEDDING APPROACHES FOR THE COMPUTATIONAL SPECTROSCOPY OF COMPLEX SYSTEMS: STATUS AND PERSPECTIVES

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The computational modeling of molecular spectra of complex systems interacting with an external environment is particularly challenging. In fact, it requires at the same time an accurate modeling of the response of the target to the external radiation field and a reliable account of the effects of the surrounding environment, which can hugely modify the solute's spectral features.
A recently developed Quantum-Mechanical (QM)/polarizable molecular mechanics (MM) embedding approach based on Fluctuating Charges and possibly Fluctuacting Dipoles [1] has shown extraordinary capabilities for aqueous systems, yielding calculated spectra in excellent agreement with experiments.
A brief overview of the fundamentals of this method is given, by focusing on specific issues related to the calculation of spectral responses in the context of selected applications [2]. Future perspectives, with special emphasis on the modelling of plasmonic nanostructured systems [3], will also be discussed.

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