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”EuCompChem2025-Trinari Marco-Oral” QM/MM simulations of ground and excited state spectroscopic properties of molecular systems in aqueous solution

The spectral properties of isolated molecules can differ significantly from those of the same molecules dissolved in aqueous solution [1]. Multiscale Quantum Mechanics (QM)/Classical models are highly effective in simulating solvated molecules by dividing the system into two components: the solute, treated at the QM level, and the solvent, modeled classically [2-4]. Among these approaches, QM/Molecular Mechanics (MM) methods have expanded considerably in recent decades and are now widely used to study the spectroscopic properties of solvated systems [1-3]. The success of this methodology lies in its ability to retain atomistic details of the solvent while accurately describing hydrogen bonding [1-3]. In this work, we investigate various ground state and excited state spectroscopic properties of molecular systems, like Tryptophan, in aqueous solution using fully polarizable QM/MM approaches [5], where the MM region is described using the Fluctuating Charges (FQ) and Fluctuating Charges and Dipoles (FQFμ) force fields [6-7]. The resulting QM/FQ and QM/FQFμ approaches are integrated with classical molecular dynamics simulations for an accurate sampling of both the ground and the excited state solute-solvent phase-space [1,8]. Computed results [9] are validated through a direct comparison with experimental data, demonstrating the robustness of our methodology.

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