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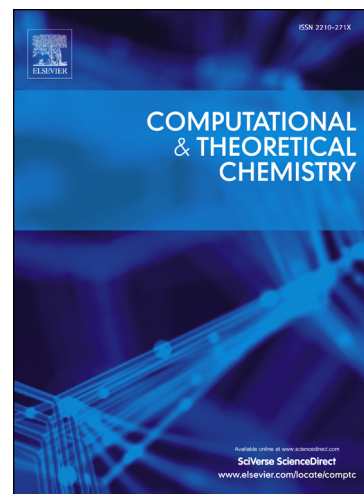
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## Theoretical Study of the Absorption and Emission Spectra of the Anionic *p*-Coumaric Methyl Ester in Gas Phase and in Solution

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### Abstract

Solvent effects on the absorption and emission spectra of the *p*-coumaric methyl ester, a model for the chromophore of the photoactive yellow protein, are analyzed using a QM/MM method known as Average Solvent Electrostatic Potential from Molecular Dynamics (ASEP/MD), which combines state of the art calculations in the description of the solute with a detailed description of the solvent through molecular dynamics simulations. Geometries for the ground and the bright excited state are optimized by using multiconfigurational (CASSCF and CASPT2) and DFT methods. Three different functionals (B3LYP, CAM-B3LYP and PBE0) were used with DFT. The effect of specific interactions and of the interplay between static and dynamic electron correlation on the spectra are analyzed. In absorption there is a flux of charge from the phenolic toward the carboxylic moiety, and the opposite is found in emission. These fluxes are similar in gas phase; however, in water solution, the flux increases with respect to the gas phase value during the absorption but not in the emission. As a consequence of these fluxes the solvent structure around the chromophore changes after the excitation. The average number of water molecules decreases around the phenolic oxygen and increases around the carbonyl oxygen. These changes in the solvent structure together the reduction of the charge on the phenolic oxygen atom during the excitation permit to explain the large Stokes shift, 0.84 eV, displayed by this system.

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