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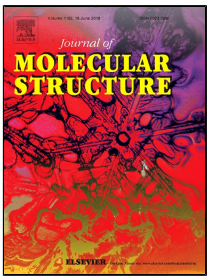

Investigation on the performance of PCM/TD-DFT functionals (standard pure, hybrid and long-range corrected) in simulating the absorption and emission spectra of 1-(2,5-dimethylfuran-3-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one dye in different solvents

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Investigation on the performance of PCM/TD-DFT functionals (standard pure, hybrid and long-range corrected) in simulating the absorption and emission spectra of 1-(2,5-dimethylfuran-3-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one dye in different solvents

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Abstract

The question investigated in this study is which functional/s of the twelve tested density functionals in combination with PCM-LR can reproduce the absorption and emission spectra of **DFTP dye** in three solvents with different polarity. **DFTP is an abbreviation of** 1-(2,5-dimethylfuran-3-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one, and **it is** with D-π-A structure. The twelve functionals range from standard pure to hybrid and long-range corrected functionals. The simulation of the experimental data included the ability to reproduce the maximum wavelength/transition energy of the absorption and emission spectra as well as the Stokes shift in CCL_4, ethanol and DMSO solvents. The geometrical parameters and dipole moments of the ground and **first excited singlet states** were compared and discussed too. The **PBE0** functional appears as the best one in reproducing the absorption, emission and **Stokes** shifts.

Keywords: Chalcone; absorption and emission spectra; TD-DFT calculations; PCM-LR

Introduction

Chalcone derivatives as electron donor-π bridge-electron acceptor are promising candidates for critical applications such as photovoltaic and materials.[1-3] Recently, one Chalcone, namely 1-(2,5-dimethylfuran-3-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one abbreviated as DFTP, was synthesized and characterized by several spectroscopic techniques [4], Figure 1. The effects of solvent polarity on the absorption and emission spectra of DFTP was investigated experimentally, and the results were interpreted regarding the intramolecular charge transfer, dipole moment and intermolecular hydrogen bonding of the ground and excited states.