Absorption and emission properties of indole by TD-DFT: what's the right functional to use?

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Indole is the aromatic side chain of tryptophan, an essential amino acid that fluoresces in the near-UV. It is used as a marker in biological systems. As detailed experiments to understand the fluorescence of Trp can be difficult to perform, we are using computational quantum methods to calculate information about Trp in its different electronic excitation states. We are testing the suitability of functionals and basis sets using time-dependent density functional theory (with Gaussian) for calculating the excitation energies, oscillator strengths, and optimized geometries of indole in several excited states. The challenge is to find a method that predicts the correct ordering of the two lowest excited states of indole and can also find distinct optimized structures of these excited states. As our research progresses, we will apply these findings to characterize the absorption and emission spectra of indole, explore the effects of a solvation on indole's fluorescence properties, and extend our work to a full tryptophan molecule.