

TD-DFT SIMULATIONS OF ORGANIC DYES

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During this talk, I will review recent successes (and failures) in the field of accurate simulations of optical spectra of medium and large organic dyes presenting a “real-life” interest. The focus will be placed on the importance of simultaneously accounting for both environmental and vibrational effects.

First, the results of TD-DFT benchmarks of the 0-0 energies, aiming to pinpoint not only the most adequate exchange-correlation functionals but also to quantify solvent effects, will be described. This will allow, on the one hand, to provide error bars for typical TD-DFT estimates of transition energies, and, on the other hand, to assess the accuracy of both TD-DFT and TDA in reproducing band shapes of organic structures. In a second step, applications performed for challenging molecules, that present transitions mixing charge-transfer and cyanine characters, will be presented. Such simulations pave the way towards efficient *ab initio* dye design of compounds in various environments.

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