TD-DFT benchmarks for organic dyes

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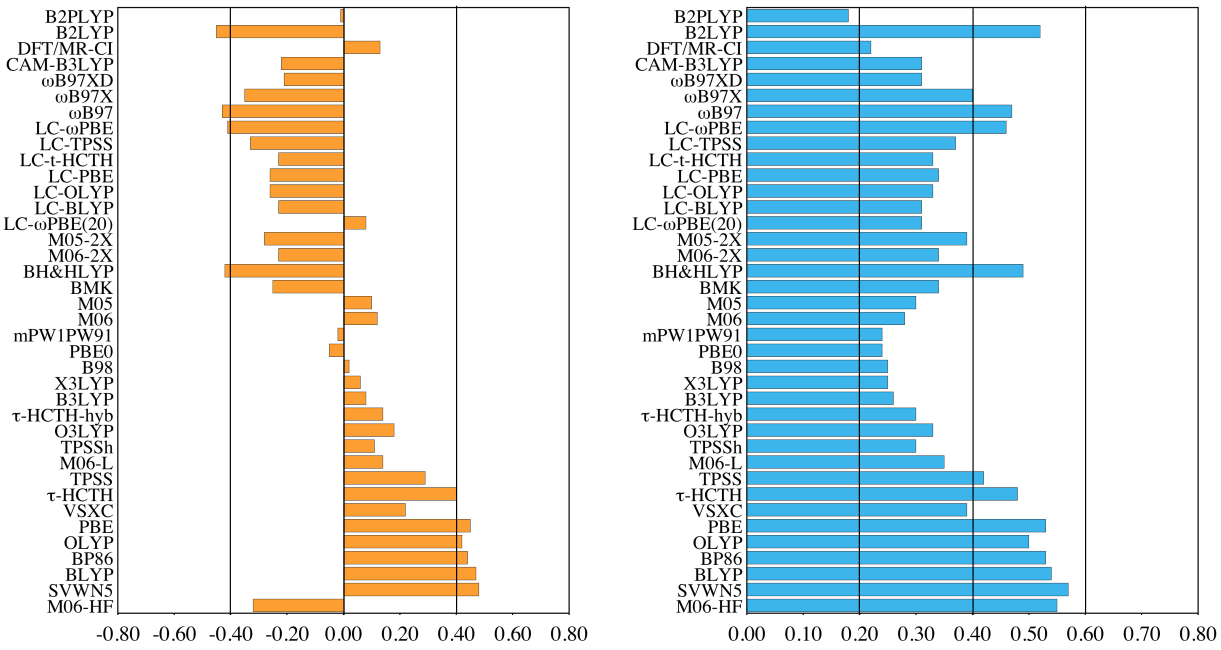
In this contribution, we summarize the results obtained with recent TD-DFT benchmarks performed on organic dyes. These benchmarks are centred on the impact of the selected exchange-correlation functional (pure, global and range-separated hybrids) on the predicted transition energies. Several families of transitions (n-π*, π-π*, singlets, triplets...) and references (theoretical or experimental) have been considered so to obtain a relatively balanced assessment of the *pros* and *cons* of each functional.



Mean signed (left) and absolute (right) deviations in eV

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