First-Principles Calculations of Excited-State Decay Rate Constants in Organic Fluorophores

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In this contribution I present computational protocols, heavily relying on DFT and TD-DFT calculations, to model excited state decay rate constants in organic fluorophores.[1] In particular, I present an extensive analysis of the models and parameters influencing the radiative rate[2] and the intersystem crossing rate constants.[3] Further, protocols to predict anti-Kasha fluorescence in molecular systems (i.e., fluorescence from higher-lying excited states)[4,5] are also presented.

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References:

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