"In-silico" Modelling of Fluorescence

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Abstract: In this contribution I present computational protocols to model fluorescence in molecular systems which go beyond the nowadays routine modelling of fluorescence energies. Our protocols merge state-of-the-art quantum chemical calculations, excited state decay rate theories (i.e., Fermi-golden rule based)[1] along with semi-classical nonadiabatic excited state dynamics to enable the quantitative determination of fluorescence lifetimes and quantum yields. In particular, I present protocols to model anti-Kasha fluorescence in molecular systems (i.e., fluorescence from higher-lying excited states)[2,3] and the first attempts to capturing fluorescence events in molecular systems within a semi-classical Non-Adiabatic Molecular Dynamics framework.[4] These investigations contribute to our continuous efforts towards attaining quantitative determinations of photochemistry at the first principles level.[5]. By treating on equal footing radiative and non-radiative processes, our methods allow to attain a complete molecular movie of the excited-state deactivation.

References:

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