Progress and challenges in the modeling of the photophysics of molecular systems: bridging experiments with theory

In this seminar I present the current progresses and challenges in the modeling of the photophysics of molecular systems with a particular emphasis on developing experimental/computational relationships. More in details, I present computational protocols developed in my research lab to model fluorescence in molecular systems which go beyond the nowadays routine modelling of fluorescence energies and oscillator strenghts.[1] 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),[3,4] but also to model intersystem crossing rate constants including Herzberg-Teller effects,[5] and the first attempts to capturing fluorescence events in molecular systems within a semi-classical Non-Adiabatic Molecular Dynamics framework.[6] These investigations contribute to our continuous efforts towards attaining quantitative determinations of photochemistry at the first principles level.[1]

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[3] K. Veys, D. Escudero, **J. Phys. Chem. A**, 124, 7228 (2020)
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[5] K. Veys, M. H. E. Bousquet, D. Jacquemin, D. Escudero, **J. Chem. Theory and Comput.**, 19, 9344 (2023).
[6] M. Pérez-Escribano, J. Jankowska, G. Granucci, D. Escudero, **J. Chem. Phys.**, 158, 124104 (2023).

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