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Two-Photon Absorption of Solvated Organic Chromophores: a Synergy between Experiment and Theory

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Abstract: Among the numerous non-linear optical processes, simultaneous absorption of two photons has gained increased attention over the last decades. This phenomenon was first predicted by Maria Göppert-Mayer in 1931 who calculated the transition probability for a two-quantum absorption process. Observation of two-photon absorption (TPA) was possible only 30 years later with the advent of lasers.
More recently, TPA has opened novel capabilities in various fields such as micro fabrication, three-dimensional optical data storage, imaging of biological tissues. This in turn has prompted the search for adequate compounds with enhanced TPA responses. Conjugated organic chromophores are good candidates, due to their inherent modularity and potential non-toxicity, and have attracted considerable interest.
Here, I will illustrate how the understanding of corresponding structure-property relationships has benefited from various theoretical approaches, including time-dependent density functional theory (TD-DFT) based methodologies. Contrarily to effective few-states models, TD-DFT is expected to provide quantitative agreement with experimental data. Yet, reaching such an agreement is still a difficult task and factors behind divergences will be highlighted. Through a couple of examples, I will show how confrontation between the experimental and the computed data gave rise to progresses.
References: F. Terenziani, C. Katan, E. Badaeva, & coll., *Adv. Mater.* 20, 4641 (2008); C. Katan, M. Charlot, C. Le Droumaguet, F. Terenziani, E. Badaeva & coll. *J. Phys. Chem. B*, 114, 3152 (2010); K. Fucke, O. Moutounet, F. Ibersiene, C. Katan & coll. *Chem Eur J.* 20,13618-13635 (2014); A. Colombo, C. Dragonetti, H. Akdas-Kilig, A. Amar, C. Katan & coll. *Dalton Trans.* 45, 11052 (2016); *Synthesis* 49(15): 3337 (2017).