Simulation of photoinduced processes and time-resolved spectroscopy by DFT

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ABSTRACT

A wide range of photoinduced reactions and far from equilibrium processes can be conveniently simulated by methods rooted in Density Functional Theory. Combining semiclassical theory, ab-initio dynamics, hybrid quantum/molecular mechanics potentials and accurate solvation methods, [1,2] we can deliver an atomistic level description of relaxation processes, photoinduced reactions and time resolved spectroscopy signals. Consequently, a detailed interpretation at the molecular level can be obtained of signals in vibrational spectroscopies (such as Femtosecond Stimulated Raman, Transient spectroscopy, multidimensional 2D Infrared), often containing a plethora of data on fs/ps time scales difficult to understand.

In this talk, we describe examples of such molecular modeling at DFT level of theory. Examples include the photo-dynamics of several photo-active systems, such as light-driven rotary molecular motors and p-stacked charge transfer complexes in solution. Other examples of applications will regard photoacids in solution and protein-DNA photoinduced crosslinking models. Perspectives will be given as conclusions.

References

[1] Coppola. F.; Cimino, P.; Petrone, A.; Rega, N., Evidence of Excited-State Vibrational Mode Governing the Photorelaxation of a Charge-Transfer Complex *J. Phys. Chem. A,* **2024**, *128*, 1620-1633.

[2] Petrone, A.; Perrella, F.; Coppola, F.; Crisci, L.; Donati, G.; Cimino, P.; Rega, N. Ultrafast photo-induced processes in complex environments: The role of accuracy in excited-state energy potentials and initial conditions, *Chem. Phys. Rev.* **2022**, *3*, 021307.