Exploring nuclear photorelaxation through an integrated ab-initio molecular dynamics and time resolved vibrational analysis approach

N. Rega[1,2]

[1] *Department of Chemical Science, University of Napoli Federico II, Complesso Universitario di M.S. Angelo, via Cintia, Napoli 80126, Italy*
[2] *CRIB Center for Advanced Biomaterials for Healthcare, Piazzale Tecchio, Napoli 80125, Italy*

In this talk we discuss a promising strategy to understand at molecular level photoinduced processes in condensed phase occurring on fast and ultrafast scale (femtoseconds to picoseconds). The approach is based on excited state ab-initio molecular dynamics simulations and a time resolved vibrational analysis to follow signals extracted from excited state trajectories.[1, 2] A hybrid implicit/explicit model of solvation, enforcing non periodic boundary conditions, is adopted to represent aqueous and non aqueous solvents.[3, 4]

Applications of photoreactions in water and non aqueous solvents will be discussed, with focus on perspectives, limits and future challenges of the method.

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