Ultrafast Population of the Benzophenone Triplet Manifold: a Photochemical Study for an Improved Understanding of DNA Photosensitization

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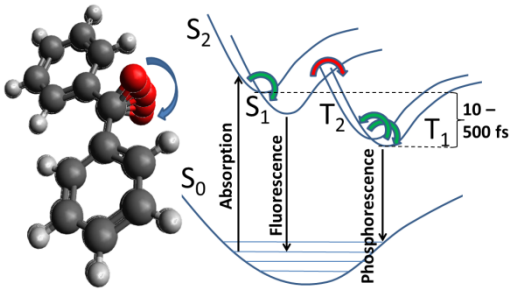
The photochemistry of benzophenone, a paradigmatic organic molecule for photosensitization processes, was investigated by means of extensive surface-hopping excited-state molecular dynamics and compared with the available experimental and theoretical data [1]. Different mechanisms were found to be relevant in the femtosecond time scale, from 10 to 600 fs: the long debated direct ($S_1 \rightarrow T_1$) and indirect ($S_1 \rightarrow T_2 \rightarrow T_1$) mechanisms for population of the low-lying triplet state are both possible, eventually allowing a kinetic equilibrium between T_1 and T_2 states never observed before, and of particular interest for benzophenone-mediated photo-induced energy transfer towards DNA [2].



References

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[2] E. Dumont, M. Wibowo, D. Roca-Sanjuán, M. Garavelli, X. Assfeld, A. Monari *J. Phys. Chem. Lett.*, **2015**, *6*, 576–580.