



**11<sup>th</sup> April 2019 - 10:00 h**

**CFEL – Building 99, seminar room I+II (ground floor)**

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## Photoactivated dynamics in DNA: from bases up to quadruplexes

Absorption of UV light by DNA, a process of fundamental biological interest, triggers a cascade of photophysical and photochemical events, which are the focus of intense research activities. On the ground of our Quantum Mechanical calculations on realistic DNA models, we shall analyse what are the most important chemical physical effects ruling these processes.[1] We shall review the basic mechanisms responsible of the photostability of the nucleobases and how their inclusion in polynucleotides gives rise to complex decay pathways. We shall focus, in particular, on the processes involving the creation or the migration of charges, which play an important role in the photoactivated dynamics of DNA.[1-5] Charge transfer (CT) excited states are formed in substantial yield via electron transfer (ET) between  $\pi$ -stacked bases in both single and double DNA strands.[2,3] In duplexes, base pairing provides the necessary reaction coordinate for interstrand proton transfer, giving rise to Proton Coupled Electron Transfer (PCET) processes, [4] which can occur also in simple hydrogen bonded pairs in low-polarity solvents.[6]

1) R. Improta et al. Chem. Rev.116, 3540 (2016). 2) Y. Zhang et al. Proc. Nat. Acad. Sci. U.S.A. 111, 11612 (2014).  
3) Y. Zhang et al. J. Chem. Phys. Lett. 7, 950 (2016) 4) Y. Zhang et al. J. Am. Chem. Soc.137, 7059 (2015). 5) A. Banyasz et al J. Am. Chem. Soc., 139, 10561 (2017). 6) L. Martinez Fernandez et al. Chem. Phys. 515, 493 (2018).

