

Quantifying photoinduced electron transfer in RNA and DNA

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Photoinduced electron transfer (PET) is one of the most fundamental phenomena responsible for the conversion of light into chemical reactions. It is also one of the most common photophysical processes occurring in UV-excited nucleic acids. It leads to the population of long-lived excited charge transfer (CT) states, characterized by quantum yields strongly dependent on sequence. However, the exact origins of this dependency remained largely obscure until recently. In this talk, I will demonstrate how quantum chemical calculations can support the discovery of new types of photoredox reaction types and prebiotically plausible pathways to RNA and DNA nucleosides under the conditions of early Earth [1,2]. I will also discuss how nucleobase sequence, stacking overlap and weak interactions modulate electronic couplings and energies of key CT states [3, 4]. These discoveries of productive photoredox reactions and nonenzymatic self-repair pathways in RNA and DNA allowed us to propose an alternative DNA nucleobase, which can substantially enhance the photostability of DNA oligomers [5, 6]. Finally, I will show our recent developments of nonadiabatic transition state theory which enable accurate prediction of photoinduced electron transfer timescales in organic chromophores [7].

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