Photostability of Uracil affected by RNA environment or shaped light

Daniel Keefer, Sebastian Reiter, Thomas Schnappinger and Regina de Vivie-Riedle

Department Chemie, Ludwig-Maximilians-Universität, München
Regina.de_Vivie@cup.uni-muenchen.de

Uracil is a key unit of nucleotides in RNA, and thereby one of the crucial players in processing genetic information. As other genetic materials it is susceptible to light, which can lead to unwanted modifications within the chemical structure and finally to photodamage. In the present work, we will use light to investigate to which extend the inherent molecular properties of Uracil, like its photostability, can be influenced and whether it can be connected to the response of Uracil to fluctuation in its the natural environment.

Quantum optimal control theory is used to design laser pulses, either to accelerate or to delay the passage towards the conical intersection between S_2- and S_1-state from where the fast relaxation to the groundstate starts. Our results demonstrate how both can be achieved [1]. When Uracil is embedded in its natural RNA environment we observe similar features. For this purpose, we employ an approach that combines wavepacket dynamics with molecular dynamics [2,3]. The influence of different combinations of neighboring nucleobases on the photostability of Uracil is discussed. While mostly the relaxation time corresponds to the gasphase situation, sometimes significantly delayed lifetimes emerge, comparable to the previously light induced changes. To the further inspect the role of the correlated electron nuclear dynamics at the S_2/S_1 conical intersection, we further investigate its controllability via CEP control induced by a few cycle pulse.

References

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