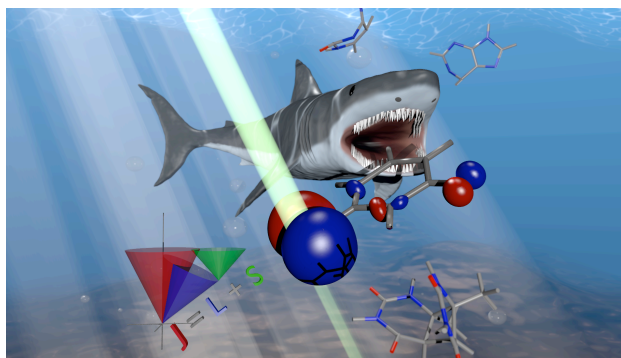


From photostability to photodamage in DNA: insights from molecular dynamics

Leticia GONZALEZ

Institute of Theoretical Chemistry, University of Vienna, Währingerstr. 17, 1090 Vienna, Austria

DNA (and RNA), as well as its constituting nucleobases, are photostable. This means that after electronic excitation by light irradiation, the system is able to return very efficiently to the electronic ground state avoiding dangerous excited state reactions. This is presumably one of the mechanisms nature has chosen to protect the genetic code from being damaged by harmful UV radiation. In general, it is agreed that the efficient relaxation of nucleobases is due to ultrafast internal conversion processes mediated by conical intersections.¹ Using a recently developed molecular dynamics code (SHARC) able to treat non-adiabatic and spin-orbit couplings on the same footing,² the dynamical processes taking place in pyrimidine nucleobases have been revisited, finding that intersystem crossing is also competitive to internal conversion. Despite efficient relaxation, in some cases, UV-photodamage takes place. The formation of cyclobutane pyrimidine dimers is one of the most abundant DNA photolesions, producing sunburn and eventually skin cancer. In this talk, our current efforts to understand the relaxation processes of nucleobases and pyrimidine dimers will be exposed.



1. S. Mai, M. Richter, P. Marquetand, and L. González, "Excitation of Nucleobases from a Computational Perspective II: Dynamics" in M. Barbatti, A. C. Borin, S. Ullrich (Eds.): Photoinduced Phenomena in Nucleic Acids. *Topics in Current Chemistry*, **355**, 99–153 (2015).
2. M. Richter, P. Marquetand, J. González-Vázquez, I. Sola, and L. González, *J. Chem. Theory Comput.* **7**, 1253–1258 (2011).

Thanks to:

