Nonadiabatic dynamics including intersystem crossing

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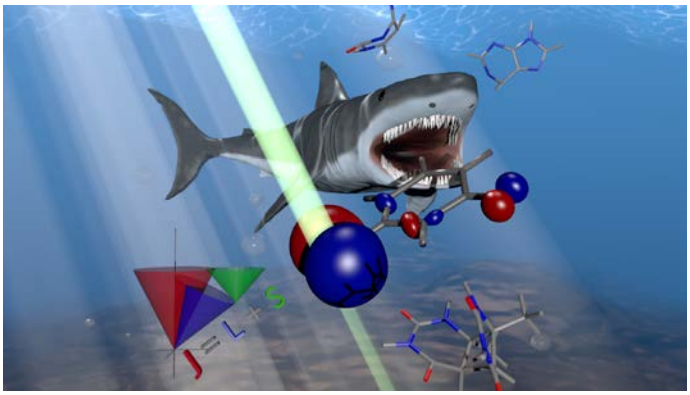
When molecules are electronically excited they can undergo photochemical reactions, exploring different regions of the excited potential energy surfaces. The description of excited state processes is considerably more complicated than ground state chemical reactions because molecules electronically excited can show a high density of states and because potential energy surfaces of same or different multiplicity can cross, breaking the Born-Oppenheimer approximation. Understanding photochemistry also requires a time-dependent analysis of the molecular pathways that a system can follow. In this presentation I will show several examples of photochemical pathways followed after light irradiation revealed with ab initio surface-hopping molecular dynamics. To that aim the locally developed ab initio molecular dynamics code (SHARC) [1], which allows treating on the same footing non-adiabatic and spin-orbit couplings, is employed.



References:

[1] M. Richter, P. Marquetand, J. González-Vázquez, I. Sola, and L. González. "SHARC - ab initio molecular dynamics with surface hopping in the adiabatic representation including arbitrary couplings". J. Chem. Theory Comput., 2011, **7**,1253-1258.