

Xing Da Lecture 596

Molecules and Light: Challenges for Theory



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1994 B.S., Autonomous University of Madrid

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1999-2007 Assistant Professor, Free University of Berlin

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Abstract

How do molecules interact with light? While light is the driving force behind a number of chemical reactions vital in chemistry, biology and even medicine understanding how molecular properties change upon light irradiation is not an easy task. Quantum theory possesses the fundamental equations to model electronically excite states and its time-evolution and yet it is plagued of challenges. In this talk I will review recent progress and strategies developed in my group to disentangle light-induced processes related to systems of different complexity, from gas phase to solution or embedded in biological environments.

Selected Publications

1. S. Mai, P. Marquetand, L. González: Nonadiabatic dynamics: The SHARC approach. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* 8, e1370, (2018),
2. S. Mai, L. González: Unconventional two-step spin relaxation dynamics of $[\text{Re}(\text{CO})_3(\text{im})(\text{phen})]^+$ in aqueous solution. *Chem. Sci.* 10, 10405-10411, (2019),
3. L. M. Ibele, P. A. Sanchez-Murcia, S. Mai, J. J. Nogueira, L. González: Excimer Intermediates en Route to Long-Lived Charge-Transfer States in Single-Stranded Adenine DNA as Revealed by Nonadiabatic Dynamics. *J. Phys. Chem. Lett.* 11, 7483-7488, (2020),

Honors and Awards

Member of tntum Molecular Sciences, Robert Bunsen Award, Dirac Medal of "World Association of Theoretical and Computational Chemists", Spanish Royal Society of Chemistry SIGMA-ALDRICH Award, Alexander von Humboldt Fellowship.