Post-Doc 2022-2023

Modeling Non-Adiabatic Dynamics: from Photochemistry to Attochemistry

Description: Post-doc position in theoretical chemistry for 18-24 months (depending on experience). Financed by the ANR Tremplin-ERC program.

Location: Team: **ModES** (Modeling & Spectroscopy)
Lab: CEISAM, UMR 6230, Nantes Université, CNRS
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CONTEXT

The applications of photochemical processes are very important (molecular switches, fluorescent probes, etc.). However, they are limited by the quantum yield of the desired process, the latter being almost always in competition with other processes. A challenge for chemists is therefore to design more efficient molecular systems as well as controlling methods for each of the applications. In this context, it is necessary to rely on a thorough knowledge of the photochemistry of the system. Time-resolved experiments with a femtosecond resolution (1 fs = 10^{-15} s) played a major role in understanding chemical reactions by probing the motion of nuclei in real time. Recent advances in attosecond science (1 as = 10^{-18} s) open the possibility of observing the motion of electrons on their intrinsic timescale. Because of the time-energy uncertainty principle, pulses of extremely short duration have a large spectral bandwidth, and can therefore be used to populate several electronic excited states in a coherent manner; this is referred to as an "electronic wavepacket". The nature and potential of chemical reactions induced by such electronic wavepackets remain largely unknown. In this field where the experimental results are still very piecemeal, theoretical studies allow not only to propose reaction mechanisms rationalizing the observed quantum yields but also to suggest better candidates as well as new means of control.

RESEARCH PROGRAM

The objective of this post-doc is to understand the photochemical and photophysical processes of organic molecules using the tools of theoretical chemistry and to work on a proof-of-concept of attochemistry to effectively control the photoreactivity of polyatomic molecules. The post-doc fellow will simulate the non-adiabatic dynamics after photoexcitation by populating either a pure adiabatic electronic state (as in traditional photochemistry) or a coherent superposition of several electronic states (attochemistry). To this end, multi-reference electronic structure and semi-classical or quantum on-the-fly ab initio molecular dynamics methods (such as the surface hopping and the DD-vMCG methods) will be used and their results will be compared. For attochemistry, an exact description of electronic coherence is expected to be crucial in the description of a chemical reaction induced by an electronic wavepacket. This post-doctoral work will imply both methodological developments and applications.

PROFILE OF THE CANDIDATE

The candidate should have obtained his/her PhD in theoretical chemistry or physics. A strong background in electronic structure and non-adiabatic dynamics methods is a highly desirable asset. Programming skills are greatly appreciated. The candidate must be motivated, show initiative and be able to work both independently and in a group. Recognized communication skills are also welcome.

Applicants must send a CV and a cover letter to morgane.vacher@univ-nantes.fr.