PhD 2024-2027

THEORETICAL ATTOPHOTOCHEMISTRY

DESCRIPTION: PhD position in theoretical chemistry: 3 years from Oct. 2024.
Doctoral contract financed by the ERC Starting Grant ATTOP.

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

One of the most fundamental and widespread processes in chemistry is the absorption of light to excite electrons of molecules and potentially induce a chemical reaction. As a result of excitation into an electronic excited state, the distribution of electrons and thus the reactivity of the molecule differ significantly from the ones in the ground state. Thanks to this conceptually simple yet complex process, photochemistry has considerably broadened the spectrum of possible reactions, as compared to thermal chemistry. Despite the current applications of photo-induced processes in many fields, the practical use of photochemistry is limited by the quantum efficiency of the desired process, the latter being almost always in competition with other processes. A challenge for chemists today is therefore to design more efficient molecular systems and optical control methods for each desired application.

RESEARCH PROGRAM

This PhD thesis is part of the ERC project ATTOP which started in October 2022. ATTOP is a theoretical chemistry project which proposes to bring the recent technological progress in attosecond science to the field of photochemistry. Light pulses of such short duration have a large spectral bandwidth and excite multiple electronic excited states in a simultaneous and coherent manner. This superposition, called an "electronic wavepacket", has a new electronic distribution and is thus expected to lead to a new chemical reactivity. The goal of the project is to investigate attophotochemistry for model systems. This requires an exact treatment of electronic coherence and thus very accurate dynamics methods. The task will be first to simulate the photochemical reactions induced by individual electronic states separately, and finally by a coherent superposition of them. The target is to propose an electronic wavepacket that increases significantly the photoreaction yield. Another aim is to learn from the specific simulated reactions and to develop general intuition rules for the new field of attophotochemistry. Visual analysis of the electron cloud of an electronic wavepacket, together with chemical know-how, should in principle indicate whether the electronic density of an electronic wavepacket has the proper shape to direct the nuclear motion in the desired direction. A direct analysis of the output of a quantum chemistry calculation for the infinite number of possible electronic wavepackets would be tedious, time-consuming, and subject to personal bias. A number of tools have been developed to automate and quantify the analysis in traditional photochemistry. The objective here is to develop new descriptors dedicated to electronic wavepackets and to use them to assess the suitability of an electronic wavepacket for a desired chemical reaction.

PROFILE OF THE CANDIDATE

The candidate should have a Master degree in chemistry, chemistry-physics, theoretical chemistry or physics, or equivalent obtained in 2023 or in 2024 and must have a solid training in physical and theoretical chemistry. Experience in *ab initio* molecular calculations as well as programming skills (Fortran, Python...) are assets.

Applicants must send a CV, a cover letter and the names of two reference persons.