Post-Doc 2021-2022

ATTOSECOND QUANTUM DYNAMICS

DESCRIPTION: Post-doc position in theoretical chemistry for 18 months.
Financed by the region *Pays de la Loire* via the project "*Etoile Montante* : ChimATTO".

LOCATION: Team: **ModES:** Modeling & Spectroscopy
Lab: CEISAM, UMR CNRS 6230 Université de Nantes
https://ceisam.univ-nantes.fr/en/

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This post-doc is part of the ChimATTO regional project that aims to develop quantum dynamics methods to be applied to attosecond dynamics. Recent technological progresses have opened up the possibility of generating light pulses of attosecond (1 as = 10^{-18} s) duration. 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. This is the application goal of the present post-doc position.

Theoretical studies complementary to the attochemistry experiments are necessary; this is all the more true in attosecond science where the information obtained experimentally is still very fragmented. There are several variants of theoretical methods to simulate non-adiabatic dynamics. Here, an exact description of electronic coherence is crucial in the description of a chemical reaction induced by an electronic wavepacket. Very accurate dynamics methods are thus required.

The major task will be to develop a methodological protocol allowing to simulate fully quantum mechanically the coupled electron and nuclear dynamics happening upon population of an electronic wavepacket in polyatomic molecules. Several methods (MCTDH, DD-vMCG, AIMS, etc.) will be investigated. This post-doctoral work will imply both methodological developments and implementations in quantum dynamics package(s).

This post-doctoral position will imply everyday collaboration with a PhD student recruited to work on applications to attosecond dynamics.

The candidate should have obtained his/her PhD in theoretical chemistry or physics. A strong background in 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, cover letter and two reference letters to morgane.vacher@univ-nantes.fr.