CEISAM
Chimie et Interdisciplinarité Synthèse, Analyse, Modélisation

UNIVERSITÉ DE NANTES
FACULTÉ DES SCIENCES ET TECHNIQUES

cnrs

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
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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 the chemical reaction induced by such an electronic wavepacket remains outstanding. There are several variants of non-adiabatic dynamic methods, the most common being the surface hopping method. Its limits are the classical treatment of the nuclear motion and the non-exact description of electronic coherence. The latter point is however crucial in the description of a chemical reaction induced by an electronic wavepacket. More 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. Several methods (MCTDH, DD-vMCG, AIMS, etc.) will be investigated. This post-doctoral work may 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 in a recognized group. A strong background in both the development and implementation of theoretical methods, and more specifically of quantum dynamics methods, is a highly desirable asset. The candidate should be motivated, show initiative and an ability to work both independently and in a group. Recognized communication skills are welcome.

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