CALL FOR 13 MONTHS OF POSTDOCTORAL POSITION IN THEORETICAL ATMOSPHERIC CHEMISTRY

Unravelling the atmospheric degradation of emerging contaminants using molecular simulations

KEYWORDS

Atmospheric chemistry, contaminants, molecular simulations, reactivity

PROJECT

The presence of atmospheric contaminants results either from direct emission from point sources: incineration, use of fossil fuels, industrial activities, etc., or from diffuse emissions or re-emissions from contaminated soils or waterbodies. This phenomenon concerns a great diversity of molecules, which originate from human activities that release volatile organic compound, containing various heteroatoms, constituting a large category of emerging contaminants (pesticides, plastics, tire wear additives, PFAS, etc.). For many of them, the atmospheric pathway is their main mode of dispersion.

The primary route for the removal of contaminants from the atmosphere is through dry or wet deposition techniques. The chemical reaction initiated by atmospheric oxidants (OH, O3) are responsible for their transformation in the atmosphere. The products formed from these reactions may be hazardous and may lead to several negative implications. Deposited atmospheric fluxes of contaminants and their corresponding degradation products also constitute an ecological risk for marine or terrestrial hydrosystems, apart from the potential human health risk due to their presence in ambient air.
The main goal of this post-doctoral fellowship is to investigate their atmospheric degradation processes using different theoretical approaches unravelling their most favourable pathways and their atmospheric fate and impact to the environment. As an add-on, the evaluation of the ecotoxicity for organic contaminants will be carried out in the aqueous environment.

QUALIFICATIONS

The candidate should have a PhD in physical chemistry, environmental chemistry, computational science or equivalent with a strong focus on theoretical or computational chemistry. Experience in the field of atmospheric chemistry, molecular simulations (quantum chemistry, molecular dynamics) and chemical kinetics is strongly recommended. Experience with relevant software packages (e.g., Gaussian, CP2K, MESS, Polyrate) will be appreciated. A good level of English (written/spoken) will be essential (at least B2).

APPLICATION

Candidates are invited to submit their application by email before March 31st 2025. The application should include a statement of research activities, a cover letter, a CV, as well as name and address of two referees who could provide a recommendation letters. Selected candidate(s) will be interviewed on site or remotely by videoconference until the application's deadline.

SALARY

Around 2200 € per month net salary before taxes

DATES

The candidate should be available to start in June 2025.

LABORATORY LOCATION

Laboratoire PhysicoChimie des Processus de Combustion et de l'Atmosphère (PC2A), UMR CNRS 8522, Villeneuve d'Ascq, France

CONTACT

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