

## Master 2: Research Training 2024-2025

Laboratory: PC2A

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Eventually CaPPA Work Package: WP-1 From gas phase to aerosols

### **Oxidation of PFAS by hydroxyl and sulfate radicals: kinetic insights from molecular simulations**

#### Abstract

Per- and polyfluoroalkyl substances (PFAS) are a class of thousands of synthetic compounds that have been widely used worldwide since the 1940s due to their ability to repel both grease and water, and to their stability towards chemical and microbial degradation. The last property, which is due to the strong C-F bond, has also had the consequence that PFAS are very persistent when released into the environment.

PFAS are introduced into the atmosphere from a large number of sources and via several mechanisms depending on their physical and chemical properties. Once in the atmosphere, PFAS undergo transport in both the gas phase and particle phase, resulting in PFAS deposition and contamination in remote regions far from the sources, as e.g. it has been observed in the Arctic regions for the past 20 years. The main goal of this internship is to investigate their atmospheric degradation processes using different theoretical approaches unravelling their most favorable pathways and their atmospheric fate.

This project will be performed within the framework of a larger research program (CPER Ecrin; Labex CaPPA, and CDP AREA). The internship will take place at PC2A laboratory, Lille University.

**Key words:** atmosphere, molecular simulations, reactivity, PFAS, environment