

International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory: PhLAM

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Eventually,

CaPPA Work Package: WP-2 Aerosol properties

Theoretical study of the ozonolysis of maleic acid droplets

Aerosols are a major component of the Earth atmosphere whose impact on climate change is not well known. Indeed, according to the last IPCC report, these particles could have a cooling effect which could counteract the observed global warming trend. Due to their complexity and diversity, the uncertainty margin is however quite large and a better knowledge of their physical and chemical properties is **needed**.

The goal of the research training is to study theoretically the ozonolysis reaction of aerosol droplets containing a small dicarboxylic acid, namely maleic acid in varying concentration and acidity conditions. To this end, two classes of methods will be employed: Molecular Mechanics (MM) methods, based on Newtonian classical theory, and Quantum Mechanics (QM). The classical approach will provide structural insight on the particle while quantum methods are mandatory to model chemical reactions. The simulation will be performed on High Performance Computers (HPC) on both local and national computing centers.

Key words: numerical simulations, electronic structure, molecular dynamics, aerosol, maleic acid