



International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory: PhLAM

Supervisor: Céline Toubin

Tél : 03.20.43.43.80 E-mail : celine.toubin@univ-lille.fr

CaPPA Work Package: WP1. From gas phase to aerosols

Molecular level investigation of organics at the air/water interface

The presence of organics at the air/water interface influences, either facilitating or inhibiting, its ice nucleation ability. In particular, this property is driven by the ability of the organics to form hydrogen bonds with the water molecules.

Classical molecular dynamics simulations can be used to complement laboratory experiments and provide indeed a molecular level description of the organization of the organics at the interface. In particular, the presence of hydrogen bonds at the interface can be monitored at different organics concentrations and temperature conditions.

We propose to first focus our efforts on two organics, resorcinol and orcinol at an aqueous solution. The student will acquire the basic knowledge on force-field based classical molecular dynamics and will learn how to use a standard package. Finally, the results from the calculations may be confronted to experimental data.

Required skills for the applicant:

Knowledge in physical chemistry.

Motivation for a theoretical work implying computer modeling.

Key words: organics, interface, hydrogen bonds, orientation, organization, classical molecular dynamics