International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory:PhLAM

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CaPPA Work Package: WP-1 From gas phase to aerosols (for example)

# Probing pyruvic acid at water/vapour interfaces with multiscale molecularmodelling

Pyruvic acid is present in the atmosphere as a product of the atmospheric oxidation of isoprene and other hydrocarbons as well as other organic species (e.g. cresol) present in the urban air, and it is one of the most abundant ketoacids found in the troposphere. Pyruvic acid has several isomers that are in equilibrium with their protonated forms.

The fate of pyruvic acid forms in the atmosphere is partly connected to their behavior at liquid water/vapor interface, making it important to characterize the predominant forms, and quantify the pyruvic protonation reactions. X-ray photoelectron spectroscopy (XPS), which can probe the C(1s) core molecular orbitals, is a surface-sensitive approach that is ideally suited to investigate processes at interfaces and to discriminate neutral from charged species.

This internship will involve the computation of C(1s) spectra for the various forms of pyruvic acids. To this end pyruvic form/water small clusters will be sampled along molecular dynamics trajectories made available by our collaborator. This reliable statistical set of structures will be post processed with the equation-of-motion coupled cluster (EOM-CC) method to compute the C(1s) core spectra combined with multiscale models of the water molecules. These spectra will be then compared to experiments. Within the project, the student will get acquainted to multiscale quantum chemical models and with the use of high-performance computing (HPC) resources.

Key words: ketoacids, relativistic electronic structure, XPS, HPC simulations