Université de Lille FACULTÉ DES SCIENCES ET TECHNOLOGIES Labex CaPPA

International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory: PhLAM

Supervisor: SEVERO PEREIRA GOMES Andre

Tél : 03.20.43.41.63, E-mail : andre.gomes@univ-lille.fr

Collaborator: DI REMIGIO Roberto

CaPPA Work Package: WP-6 Hazard: dispersion, reactivity, deposition of radionuclides

Assessing new electronic structure methods for computational X-ray spectroscopy of halogenated species at interfaces

Aerosols are ubiquitous in the air we breathe and have been recognized to have a significant impact on our society, through their adverse effects on climate and public health. Among these, those containing halogens are particularly interesting: while for the most part such aerosols are of marine origin (sea salt), the release of radionuclides (iodine) in the environment due to industrial accidents may also be of importance. The interaction of such elements with particles (dust, ice, droplets) may induce physico-chemical changes that could, for instance, modify their bioavailability.

Chemical and physical processes taking place at interfaces, such as air/solid (molecules on ice or dust particles) or air/liquid or liquid/liquid (species on droplets), however, are still poorly understood. X-ray photoelectron spectroscopy (XPS), which probes the ionization of core molecular orbitals, is a surface-sensitive approach that is ideally suited to investigate processes at interfaces. Experimental data are very complex and for its interpretation input from theoretical models (e.g. from ab initio electronic structure calculations) is essential.

This internship will involve the assessment of novel electronic structure methods, combining the highly accurate equation-of-motion coupled cluster (EOM-CC) method for core states combined with multiscale approximations for the ice surface. Within the project, the students will explore the effect of relativistic corrections and that of different models for the ice surface, and be acquainted with the use of high-performance computing (HPC) resources.

Key words: relativistic electronic structure, embedding methods, XPS, simulations