International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory: PhLAM

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CaPPA Work Package: WP1. From gas phase to aerosols

Understanding the core ionization spectra of iodated species in solutions via computational X-ray spectroscopy

The behavior of iodine-containing molecules is central to the understanding of (photo)chemical reactions taking place at the marine boundary layer (MBL). Among many species present, methyl iodide (CH_3I) takes a central place as it is the most abundant compound found in the MBL. A thorough understanding of the behavior of CH_3I at the air/liquid and liquid/liquid interfaces is therefore of great value for a better understanding of its affinity for the different media.

X-ray photoelectron spectroscopy (XPS), which probes the ionization of core molecular orbitals, is a surface-sensitive approach that is ideally suited to experimentally investigate processes at interfaces. Due to the complexity of the underlying processes, however, the interpretation of XPS spectra required information from theoretical models, as provided by electronic structure calculations.

This internship will involve the use of equation-of-motion coupled cluster (EOM-CC) method to determine the core ionizations of CH_3I in aqueous phase, in combination with the frozen density embedding method to efficiently describe the effects of the environment. Due to the importance of relativistic effects for the core levels of species such as I, the student will be exposed to relativistic electronic structure theory.

Key words: Iodated complexes, XPS, relativistic ab initio calculations