

## jj International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory: PhLAM

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CaPPA Work Package: WP-6: Radionuclides - their fate

### Probing Actinides properties via quantum chemical approaches

The subject of this internship is centered on the study of the elements involved in the nuclear cycle and more particularly those which will be at the heart of the problems of storage and recycling of used fuel (radionuclides: RN). Our main objective is to increase fundamental knowledge in terms of physical chemistry on these highly radioactive elements for some, which will help to improve future recycling facilities. Due to the strong experimental constraints linked to the dangerousness of these elements, their study requires having specific installations. In addition, for some, data such as constants of complexation, enthalpies of formation are non-existent, or incomplete, as well as the characterization of the spectroscopic properties.

In addition to these experiments, quantum chemistry methods are best suited to describe, understand and predict the properties of these elements, which are strongly dependent on the interaction between RN and the ligands present in the RN vicinity.

In particular, we propose to first focus our efforts on the properties of Cm(III) ion.

The student will start to learn QC package which can probe the various properties of these elements and generate data that will be confronted to experimental data not available yet.

The possible follow-up of this master project is to acquire the missing experimental data within a PhD in "cotutelle" with our experimental collaborators located in Germany (HZDR Dresden) and to develop a joint approach combining simulations and experiments.

#### **Required skills for the applicant:**

Knowledge in physical chemistry. Motivation for a theoretical work implying computer modeling. Calculations will be carried out in a Linux environment using standard electronic structure packages and coding specific analysis programs.

**Key words:** Quantum Chemistry, Actinides, Spectroscopy