Title of post: PhD student to develop a CHON+PS chemical scheme validated at high temperatures with applications in planetology.

General Information:
Workplace: Laboratoire Interuniversitaire des Systèmes Atmosphériques in Créteil (France) and at the Laboratoire Réactions et Génie des Procédés in Nancy (France)
Publication date: 20 July 2021
Name of the Scientific Leader: Olivia Venot
Type of contract: Doctoral student/Doctoral contract
Expected start date: 1 November 2021
Contract duration: 36 months
Working hours: Full time
Remuneration: 2135,00 € gross monthly
Level required: M2 / Engineer

Missions:

Context: To learn more about the fascinating new worlds of exoplanets, several space telescopes have been designed, such as the JWST (James Webb Space Telescope, launch in October 2021) and Ariel (Atmospheric Remote-sensing Infrared Exoplanet Large Survey, launch in 2029). The broad wavelength coverage and high-sensitivity of the instruments on-board these telescopes will allow us to extract much more information from their data than what has been possible so far, leading to numerous breakthroughs. However, these breakthroughs will be possible only if the models used to interpret the high-resolution observations are robust and reliable. In particular, photo-thermochemical models calculate the chemical composition of exoplanet atmospheres, taking into account the particular chemistry occurring in these media and the effect of disequilibrium processes. The main ingredient of these models, the chemical scheme has to be specifically tailored for their extreme conditions, that is to say very high temperatures and pressures. Thanks to a close collaboration between the Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA) and the Laboratoire Réactions et Génie des Procédés (LRGP), we are the only team in the world capable of providing highly reliable chemical schemes validated over combustion experiments (Venot+2012, 2015, 2020). These schemes, containing Carbon, Hydrogen, Oxygen, and Nitrogen species (CHON) are made available to the community through the KIDA Database and regularly downloaded. However, for a more reliable simulation of exoplanet atmospheric composition, significant improvements are still required: Sulfur- and Phosphorous-bearing molecules can affect the observations of exoplanets' atmospheres and thus need to be incorporated in atmospheric models that are used to analyze them. Within the ANR project "EXACT (EXoplanetary Atmospheric Chemistry at high Temperature)", the hired PhD candidate will develop a comprehensive CHON+PS scheme and will apply this newly developed scheme to the study of exoplanetary atmospheres, using a kinetic model.

Objective: During the first part of the PhD (18 months), the student will develop the CHON+PS scheme, starting from our most up-to-date CHON scheme (Venot+2020). The scheme will be validated through experimental measurements over a large range of pressures (0.01-500 bars) and temperatures (300-2500 K). This development will be performed at LRGP with internationally-recognized experts in experimental and modelling study of combustion kinetics. During the second part of the PhD (18 months), the student will apply the newly developed scheme to the study of planetary atmospheres, using a kinetic model. This work will be performed at LISA with experts in modeling of (exo)planetary atmospheres.
The PhD student will be co-supervised by Olivia Venot at LISA and Baptiste Sirjean at LRGP.

Activities:

The primary tasks of the PhD fellow are:
- Bibliographical work
- Drive the development and validation of CHON+PS kinetic models
- Develop methods, using computational chemistry, to calculate and tabulate gas-phase rate constants
- Adapt the existing chemical kinetic code to the newly developed scheme

- Develop atmospheric models for various exoplanets and study the chemical composition
- Evaluate the detectability of the new S- and P-species on synthetic spectra
- Writing of scientific articles and thesis and disseminate research results at conferences and seminars.

Skills:

We are looking for an extremely motivated student who will be fully involved in a challenging interdisciplinary project linking the fields of combustion and astrophysics. The PhD candidate will have a double expertise, both in chemical schemes development and in atmospheric modeling. This unique formation will guarantee him/her an unprecedented interdisciplinary profile. Desired profile: *i)* Either a Master or Engineer degree in organic chemistry, chemical engineering, chemistry, physics or related fields with a great interest for astrophysics, in particular exoplanets, or a Master degree in Astrophysics, with a strong background on chemistry, chemical engineering; *ii)* Good English skills to work in an international environment; *iii)* Good programming skills.

Context of work:

The PhD program takes place within the ANR JCJC project "EXACT" led by Dr Olivia Venot. The PhD candidate will work at the LRGP during the first 18 months of the PhD and at the LISA during the other 18 months. In these two labs, the PhD candidate will join active teams composed of several permanent researchers, PhD students and post-docs.

- The Laboratoire Réactions et Génie des Procédés (LRGP) is a Joint Research Unit of the CNRS and the University of Lorraine. It is located in Nancy, France's second biggest student city. It is mainly located in the city center, in the premises of the National School of Chemical Industries of Nancy (ENSIC). The research lab is a leading chemical and process engineering laboratory in France and in the world. The PhD candidate will work within the Radical Kinetics Group, which has an international recognized expertise in combustion kinetics, both on the experimental and modelling sides. Existing experimental devices to study these phenomena include shock tube, laminar flames and jet-stirred reactor experiments. Numerical tools include Gaussian16, Chemkin Pro, COSMO-RS and other similar codes.

- The Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA) is a Joint Research Unit of the CNRS, the Université Paris-Est Créteil, and the Université de Paris. It belongs to the Observatoire Des Sciences de l'Univers EFLUVE and to the Research Federation IPSL. It is located in Créteil, an important student city in the Paris region. The research lab is a leader in atmospheric modeling at the international level. Its main mission is to contribute to improving our knowledge of the functioning of the Earth's and planetary atmospheres in order to understand their past evolution and predict their future trajectories. The PhD candidate will join the Exobiology and Astrochemistry group, whose main objectives are the search for molecular structures and the study of the various physico-chemical processes governing the chemical evolution of various astrophysical objects (exoplanets, comets, Mars, Titan…). They are internationally recognized as world class experts in planetary atmospheres from both a modeling and experimental point of view. They are strongly involved in the analysis of observational data from ground-based facilities and space missions.

We offer: a multi-disciplinary formation and training using state-of-the-art research equipment, participations in national or international schools, conferences and workshops. The PhD student will also follow high-level formations proposed by the Doctoral School.

Constraints and risks: Short trips abroad.

Supplementary information:

Application should be sent to Dr Olivia Venot (olivia.venot@lisa.ipsl.fr) and Dr Baptiste Sirjean (baptiste.sirjean@univ-lorraine.fr) before September, 1st 2021. Required documents should be sent in a single PDF file that includes a letter of motivation, a CV and academic transcripts of records in French or English.