

## Recruitment for a research contract : Junior Professor

Junior Professors are primarily recruited among researchers who have shown their ability to produce world-class research, confirmed by high-quality publications, with experience in project coordination and leadership, throughout their careers.

Recruitment on the basis of a research and teaching project on a fixed-term contract known as a "Junior Professor" should enable the agent access to a permanent position as a professor at the Clermont Auvergne University, after evaluation of their scientific value and professional aptitude. The probationary period is fixed to 4 years.

## Job description and project sheet

**Institution / organization:** Université Clermont Auvergne (UCA - University of Clermont Auvergne)

**Host Laboratory:** Institut de Chimie de Clermont-Ferrand (ICCF, UMR CNRS 6296)

**Contract effective date:** 01/09/2022

**Partner institutions / organizations:** *CNRS-INC*

**Title of the project:** multi-scale modelling of polymer materials

**Duration:** 4 years

**Scientific theme:** Molecular simulations of polymer materials

**Keywords:** *polymer materials, molecular simulations, structure-property relationships, polymer-liquid interactions, multi-scale modelling.*

**Research fields EURAXESS:**

Computer science: modelling tool

Chemistry: computational chemistry, physical chemistry

Physics: chemical physics, statistical physics

**Teaching and research profile:**

The junior professor will teach chemistry and physics. Research will focus on molecular simulation of polymeric materials and polymers at interfaces.

**Job profile:**

The candidate will perform their teaching duties in physical chemistry. The research activity will focus on the molecular simulation of polymeric material and polymers at interfaces by using models with different resolutions (from the molecular to the mesoscopic scales).

**Institution strategy:**

SimatLab is a joint public-private UCA-CNRS-Michelin laboratory hosted by the Clermont-Ferrand Institute of Chemistry (ICCF, UMR CNRS 6296) within the Thermodynamics and Molecular Interactions team (TIM). Part of its research activities are integrated in the Challenge 2 programme: Innovative systems and services for transport and production of the I-SITE CAP 20-25 Clermont Auvergne Project. The present junior professor position will strengthen and perpetuate this activity as part of the PIA "Excellences" call for projects (CAP REU-Site Project). In addition, the UCA wishes to expand long-term partnerships with the socio-economic world. This position will:

- strengthen the SimatLab research potential
- help to extend its activity to new themes
- broaden its collaborative field to a consortium of companies and new research units on the Clermont-Ferrand site (mathematics, physics, experimental chemistry).

**Host laboratory strategy:**

SimatLab is a joint research laboratory initially created in 2017 by the UCA, the CNRS and Michelin. It was renewed for 4 years in September 2021 with EPE-UCA, CNRS, CHU Clermont-Ferrand and Michelin as supervisors. SimatLab is hosted by the Institute of Chemistry of Clermont-Ferrand (ICCF, UMR CNRS 6296) in the Thermodynamics and Molecular Interactions (TIM) team. Over the next 4 years, the laboratory will have to develop new theoretical knowledge on the physics of scale change and new methodologies: Artificial Intelligence & Machine Learning, experimental characterizations of the energetics of adsorption and structural characterizations of interfaces. The ambition is to apply all these methods to new fields such as the biocompatibility of medical devices with the CHU and to new application subjects for Michelin such as the biodegradability of polymers, polymer membranes for fuel cell and electrolyser applications. The recruitment of the Junior Professor will therefore contribute to the multi-scale simulation activities in all its variations, to the opening up of Artificial Intelligence and to research themes in the pharmaceutical field.

**Abstract of the scientific project:**

The scientific project focuses on the passage of information from a molecular description of matter (high resolution) to a mesoscopic description (low resolution) with the aim of developing "coarse-grained" models for the modelling of polymeric materials. Numerous scientific issues remain to be overcome regarding the transferability of large-grain models: from the bulk to the interface, from the homopolymer to the copolymer, on the chemical nature of the monomer, in temperature and pressure. Introducing reactivity at the coarse-grained level will allow the study of the incorporation of reversible bonds in resins, the enzymatic degradation of polymers, and the protonic conductivity in polymer membranes. Methodological and theoretical developments will be tested on the following applications: interactions between active ingredients and polymeric surfaces, release mechanisms of additives mixed with synthetic polymers used in medical devices, design of reversible networks for durable resins, structure-property relationships of thermoplastic elastomers and enzymatic degradation of a polymer at a polymer-water interface, ionic transport in nano-structured materials.

**Abstract of the teaching project:**

The candidate recruited will teach in the Chemistry Department of the University of Clermont Auvergne. They will be expected to fully commit to teaching lectures, tutorials and practical work in Physical Chemistry at all levels of university education. In this respect, they will reinforce the teaching team, particularly in the following subjects: chemical thermodynamics, chemical kinetics, structure of matter and programming (algorithmic, language). Specific skills in molecular thermodynamics and/or polymeric materials would be highly appreciated. Expertise in the development of courses dedicated to the molecular simulation of polymeric materials would also be welcomed.

The teaching duties will include 42 hours of lectures or 64 hours of practical work or seminars.

**Scientific dissemination:**

Scientific dissemination of the joint laboratory is relatively classical concerning research valorization through the production of new scientific knowledge and new simulation methodologies, thus favoring the publication of results in international peer-reviewed journals and presentations at international conferences. The interdisciplinary dynamics and the simulation-experiments will lead to publications in journals with a wider audience. Deliverables are expected on simulation algorithms within the joint SimatLab.

### **Open science:**

The scientific activity will follow the open science policy of the UCA on making scientific production available in full version in the HAL Clermont database, within the life cycle of the date produced.

### **Science and Society:**

The SimatLab joint laboratory is already involved in scientific events such as:

- the Fête de la Science
- the scientific festival "Les Nuées Ardentes" combining art, science, and imagination
- and the "Jacques Cartier" talks.

The project therefore provides scientific communication actions aimed at the general public and/or high school and undergraduate students, but also within the framework of the SAPSAU project (Science Avec et Pour la Société en Auvergne), which will be awarded the SAPS (Science Avec et Pour la Société) label in 2022.

### **Indicators:**

The deployment of the project will be monitored through monthly scientific meetings of the joint laboratory and an annual presentation of the SimatLab results to the steering committee, which brings together laboratory sponsors (UCA, CHU, CNRS and Michelin).

### **Monitoring indicators:**

Progress of theses related to the project

Rate of transfer of methodologies to Michelin

Rate of internal use of the methods at Michelin

Valorisation of results (publications, conferences, ....)

Evaluation of the added value of interdisciplinarity

Evaluation of the number of collaborations and project applications generated by the junior professor's research

Recruitment of non-permanent staff and follow-up of their professional integration

### **2022 Campaign calendar:**

The 2022 campaign calendar calendar will be announced soon.

### **Contact:**

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