



Laboratoire de Physique et Chimie Théoriques
UMR 7019 CNRS/Université de Lorraine
Faculté des Sciences et Techniques
54506 Vandœuvre-lès-Nancy
<https://lpct.cnrs.fr>



Research engineer - Scientific computing

BAP : E - Expert in High-Performance Computing (E1E45)

✓ General information:

Employer: Centre National de la Recherche Scientifique

Job type: Civil servant

Contract duration : Open-ended contract

Starting date: 01/12/2024 (negotiable)

Working hours: Full time

Salary: depending on professional experience

Level of education required: Master's Degree

Desired experience: >1 year

✓ Context:

The Laboratoire de Physique et Chimie Théoriques - LPCT UMR CNRS - Université de Lorraine 7019 is an internationally recognized research unit currently bringing together most of Lorraine's theorists (physicists and chemists), located at the Faculty of Sciences and Techniques in Nancy and at the Institut of Physical Chemistry and Materials in Metz. The agent will be located on the Nancy site, where the computing infrastructure is housed, and may be called upon to work on the Metz site from time to time.

The LPCT's high-performance computing infrastructure consists of a computing platform with a power of over 2 petaflops (>6000 CPU cores and >200 GPU cards) and a storage system for over 1 Po of data, duplicated on capacitive storage.

✓ Mission :

The recruited person will harness mathematical and computational methods to assist researchers in the development of algorithms and the implementation/optimization/utilization of computational codes for theoretical chemistry, biochemistry and physics simulations. He/she will manage the laboratory's High-Performance Computing (HPC) infrastructure and support researchers in the use of these resources.

✓ Profil:

The recruited person, who may hold a doctoral thesis in the field of computational chemistry and physics, will need to demonstrate experience or interest in HPC/GPU and scientific computing. He/she will have skills in the use, development and compilation/optimization of scientific codes. Knowledge of HPC system administration tools is desirable. The successful candidate will need to show a willingness to adapt and learn, as well as the interpersonal skills required for teamwork. He/she must also be self-reliant and able to take the initiative.

✓ Activities:

- Support users of scientific computing tools (hardware and software).



- Provide laboratory researchers with expertise in the use of mathematical methods and computational techniques for modeling and simulation in theoretical chemistry, biochemistry and physics.
- Participate in national and international research projects and associated publications
- Manage the lifecycle of computational data, organize and monitor its use (storage, backup of data from digital simulations).
- Participate in the selection, acquisition and operation of the laboratory's HPC infrastructure
- Update the operating system of the HPC infrastructure and all calculation codes used in the laboratory.
- Manage licenses for commercial codes used by laboratory researchers
- Write and update technical documentation relating to the laboratory's computing infrastructure.

✓ **Associated activities:**

- Monitor data storage operations
- Manage relations with suppliers of software used by the laboratory's researchers and hardware suppliers
- Ensure dialogue between the LPCT and the digital services of the university and CNRS.
- Ensure dialogue between the LPCT and computing centers (in particular Datacenter of Lorraine, Computing mesocenter of Lorraine, Genci, etc.).
- Participate in the expert network of HPC engineers.

✓ **Technical skills:**

- Mathematics libraries
- Algorithmics
- Scientific computing tools in quantum chemistry, molecular dynamics, solid-state physics and mathematics (Gaussian, Molcas, Orca, ADF, Turbomole, VASP, QuantumExpresso, CP2K, Namd, Amber, Gromacs, OpenMM, Rosetta, AlphaFold, Mathematica, Octave, ...)
- HPC infrastructure management and operating systems
- Programming languages (fortran, c++, python, pearl, java, cuda ...)
- English language: B2 to C1 (Common European Framework of Reference for Languages)

✓ **Operational skills:**

- Project management
- Implement a quality policy
- Draft documents
- Support and advise
- Communicate and be educational
- Monitor technical developments

✓ **Working conditions:**

The person recruited will benefit from an adapted work environment. The weekly working time is set at 38H30 (variable hours between 7:30 a.m. and 7:00 p.m. with fixed periods (9:00 a.m. – 11:30 a.m. – 2:00 p.m. – 4:00 p.m.)). He/she will be entitled to 44 days of annual vacation. The LPCT is an equal opportunity laboratory with a working environment actively promoting equality, diversity and inclusion.



Laboratoire de Physique et Chimie Théoriques
UMR 7019 CNRS/Université de Lorraine
Faculté des Sciences et Techniques
54506 Vandœuvre-lès-Nancy
<https://lpct.cnrs.fr>



How to apply

Registration for the 2024 external competitions will be open from June 10 at 11 a.m. to July 10 at 1 p.m. (Paris time) directly on the CNRS website: <https://carrieres.cnrs.fr/en/concours-externes-des-ingenieurs-et-techniciens-h-f/>

Contact

Mariachiara Pastore (mariachiara.pastore@univ-lorraine.fr), LPCT HPC Department Manager