

## Vacancy

# Computational Scientist - Atomistic Simulations

## Your Tasks

Although you will be a member of the Scientific Computing group (CS), a significant part of your work will relate to the research topics addressed by the Spectroscopy group, which is responsible for all of the ILL's neutron spectrometers.

- IPAD Platform Development: You will support the development of the IPAD platform (Integrated Platform for Analysing Data), working closely with scientists and ILL internal teams (IT, SCI, DS) as well as external partners (University of Oslo - Hylleraas Center). This role requires a strong understanding of scientists' needs and the various aspects of neutron scattering data reduction and analysis.
- Battery Hub - Simulation Activities: You will contribute to the scientific developments within the Battery Hub, with a focus on atomistic simulations (Classical MD, Ab-initio, DFT) running on the ILL's HPC cluster. In this capacity, you will be responsible for coordinating, initiating, and supporting simulation projects within the Hub, in particular those requiring expertise in spectroscopy.
- IN1-Lagrange — User Support: You will help to develop new methods for analysing data and conducting experiments on the IN1-Lagrange spectrometer (AI-Machine Learning, Bayesian analysis, etc.). In this role, you will provide experimental support to external users of this instrument (by acting as Local Contact).

## Qualifications / Experience

PhD in physics, chemistry or a related field.

- Programming skills are essential (Python and/or other scientific computing languages), together with a solid experience of working with DFT software (such as VASP, Quantum ESPRESSO and CP2K) for the study of condensed matter.
- Knowledge of artificial intelligence, and in particular machine learning, would be an advantage.
- Experience in spectroscopy techniques (particularly vibrational spectroscopy) would be a plus.
- Knowledge of battery-related problems and materials would be welcome.

## We offer:

- ✓ **Quality of life** A hub for research and technology, the city of Grenoble is ideally located in the heart of the French Alps (just 3 hours from Paris/Provence by train, 1 hour from Lyon international airport and 1 ½ hours from Geneva). It is important for us that our staff achieve a healthy work-life balance. We therefore offer home working (under certain conditions), generous annual paid leave entitlement and a host of other benefits that you will discover when you arrive!
- ✓ **Prospects** We guarantee you a **5-year fixed-term contract** in a multicultural scientific environment.

**Benefits** - We offer generous social benefits (expatriation allowance, excellent health cover), moving and relocation assistance (under certain conditions) and an annual productivity bonus. We also offer language courses for you and your partner and subsidies for the use of public transport and the staff canteen, as well as for holidays and a variety of cultural and sports activities. For more details, visit <https://www.ill.eu/careers/working-at-the-ill/employment-conditions>

## How to apply:

[https://www.ill-recruits.eu/module.php?module=applicant\\_register\\_cv\\_analyzer/applicant\\_register\\_cv\\_upload&sid=2215](https://www.ill-recruits.eu/module.php?module=applicant_register_cv_analyzer/applicant_register_cv_upload&sid=2215)

Then why not take your next career step with us by applying online - preferably in English - via our career portal by **21.06.2026, quoting reference number 26/26** with a list of publications and the names of 3 referees, including one from your present workplace. Please note that all applicants are subject to administrative screening (background checks). For this post, medical fitness, including work under ionizing radiation, is required. We are committed to equal opportunities and diversity and therefore welcome applications from all suitably qualified candidates.

Con copia de la candidatura a: [eures.franciasuizabeneLux@sepe.es](mailto:eures.franciasuizabeneLux@sepe.es)

Indicando la referencia ILL **26/26**

## Ayudas a la movilidad EURES

