



Post-Doctoral fellowship in Electrostructure & magnetism – 18-month post-doctoral contract

Context of the mission

The objectives of the ILL Theory group are both to provide theoretical support to ILL scientists and users and to develop its own projects on neutron-related subjects. In this respect it favours long-term scientific collaborations rather than a service activity and tries to cover a wide range of scientific domains.

Our scientific activity thus covers subjects ranging from strong correlation in condensed matter to the simulation of cell membranes in biophysics. We also use a variety of techniques, from analytical methods to Monte-Carlo simulation or ab-initio electronic structure calculations.

As our aim is to be an effective support to the ILL instrument scientists and ILL users, most of our work is directly related to experimental projects. To be efficient in providing theoretical support, however, requires that we also spend some time developing new methods.

Your tasks

The goal of the mission is to work on ab-initio electronic structure and spectroscopic calculations in strongly correlated systems with a special focus on magnetic and multiferroic systems. According to his/her abilities and taste, the successful candidate will either work on specific compounds, in close collaboration with experimentalists, or on methodological developments in close collaboration with the Scientific Computing group:

- In the first case the candidate will use ab-initio methods to develop effective models able to bring a coherent understanding of the experimentally observed properties of specific compounds. A special focus will be given to the understanding of neutron diffraction data, such as magnetic structure, magnetic excitations, etc.
- In the second case the candidate will rather focus on developing methods in order to better reach the prediction of excitation spectra, in particular magnetic ones. This could mean working on developing ab-initio methods, developing an artificial intelligence replacement for the ab-initio calculations, developing the concepts and methodology to compute specific properties, etc.

Your profile

The successful candidate should have:

- A PhD in condensed matter physics or quantum chemistry.
- A strong background in quantum mechanics, a reasonable knowledge of electronic structure calculations (such as DFT, wave-function methods, etc.).
- Experience in programming languages and experience with Linux.
- Some knowledge of group theory or crystallography would be appreciated.
- Similar knowledge of modern parallelization and programming/versioning methods (MPI, OpenMP, OpenACC, Git, etc.) would be a plus.

What 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 secure 18-month post-doctoral contract, renewable for a further 6 to 18-month period. **Only candidates holding a PhD obtained less than 4 years ago are eligible for post-doctoral positions at ILL.**



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.

Sounds interesting?

Then why not take your next career step with us by applying online [HERE](#) - preferably in English - via our career portal **and** send an e-mail with your application to the Theory Group responsible : lepetit@ill.fr by **16.07.2023**, quoting reference number **23/28**, with a list of publications and the names of 3 referees, including one from your present work place. Please note that all applicants are subject to administrative screening (background checks). For this post, medical fitness for work under ionising radiation is required. We are committed to equal opportunities and diversity and therefore welcome applications from all suitably qualified candidates.

The Institut Laue-Langevin (ILL) is based in Grenoble (France) and operates Europe's leading research facility for basic research with neutrons. United by our passion for progress and technology, we drive science and research forward every day. Together, we can pave the way for discoveries that will help to make our world a better place.