



Post-Doctoral fellowship in nanofluidics

Post-doctoral contract

Context of the mission

The objectives of the ILL's 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 physical chemistry systems and cell membranes in biophysics. We also use a variety of techniques, from analytical methods to molecular dynamics and Monte-Carlo simulations to ab-initio electronic structure calculations. The project will focus on the fluid/solid interface as encountered in nanoconfined liquids, which is the locus of a wide spectrum of microscopic phenomena such as adsorption and chemical reactions. Theoretical descriptions of nanoconfined fluids – except for rare contributions – assume perfectly metallic or insulating confining surfaces, but these asymptotic limits do not necessarily reflect actual materials that correspond to imperfect intermediate metals/insulators. Nonetheless, the electrostatic boundary condition imposed by the surrounding medium affects confined dipolar systems and, even more so, charged systems [Comtet et al. Nature Mat. 2017]. Recently, we have developed an effective atom-scale simulation approach that allows us to consider the confinement between surfaces of any electrostatic screening length and geometry [Schlaich et al. Nature Mat., 2022]. The electrostatic screening induced by the confining material is modelled by the response of a high-temperature fluid composed of light ions. Due to its very fast relaxation, this virtual Thomas-Fermi fluid mimics the metal electrostatic response in the confining surfaces during the simulation of the confined system (Monte Carlo or molecular dynamics).

Your tasks

With this postdoc position, we propose to use the molecular simulation strategy recently developed to investigate the impact of the metallic surface and its underlying electrostatic relaxation on the thermodynamics and dynamics of dipolar and charged fluids. This should ultimately extend the understanding of adsorption and transport phenomena to a large class of nanoporous materials (i.e. nanoporous metals) that has received relatively little attention in terms of their confinement properties. In particular, this work could open the way to developments in catalysis (metallic surface) but also for electrochemical and electromechanical applications, etc.

While the postdoc is theoretical in nature, the work will be done in collaboration with Prof. Lydéric Bocquet's group in Paris, which has experimental/theoretical expertise on this topic. Possible collaboration with ILL scientists and/or users will be sought to build a joint task force on this topic.

Your profile

The successful candidate should have:

- a PhD in physics, physical chemistry or materials science
- a strong background in statistical mechanics and knowledge of the thermodynamics and dynamics of fluids at interfaces/in confinement.

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 - preferably in English - via our career portal by **18.06.2023**, quoting reference number **23/22**, 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.