Postdoctoral research position at Sorbonne University, Paris, France

"New routes to free energy sampling including nuclear quantum effects"

The Laboratory of Excellence (Labex) Materials, Interfaces, Surfaces and Environment (MATISSE) is pleased to announce an 18-month postdoctoral position, at the Paris Institute for Nano-Sciences (INSP), in the frame of a joint research project with the Swiss Federal Technical School (EPFL) in Lausanne, the Ecole Normale Supérieure (ENS) and the Institute of Materials Physics, Mineralogy and Cosmo-chemistry (IMPMC) in Paris.

Atomic nuclei are quantum particles, but their statistical or dynamical properties are generally treated classically as their mass is relatively large. However, even at ambient conditions, the thermal wavelength of light nuclei such as protons is not negligible with respect to inter-atomic distances. The reference method for computing statistical averages at equilibrium while including nuclear quantum effects (NQEs) is the Path-Integral Molecular Dynamics. Recently, a stochastic Langevin equation has been proposed to describe NQEs by using a frequency-dependent noise – the Quantum thermal Bath (QTB). Although exact only in the harmonic case, the QTB is a fast and versatile method that allows an effective sampling of the energy landscape incorporating NQEs in an approximate way [1,2].
We plan to combine the QTB method and techniques derived from the path-integral formalism with an efficient sampling of the free-energy including NQEs [3,4]. We aim at obtaining an accurate method that still retains the effectiveness of the QTB. Such a combination would allow treating a class of problems that are presently out of reach of first-principles molecular dynamics.

The 18 months of the postdoctoral contract will include a short starting phase that will be devoted to the development of the theoretical method and the simulation tools. Proofs-of-concepts have been already carried out during short master internships. Accordingly, the methods will be set up and tested on model systems, in order to assess their capabilities and drawbacks, before being applied to complex systems, where the atomic forces will be computed via density functional theory. In a further step, the methods will be applied to materials under high pressures as currently investigated by the experimental group of L. Bove at the IMPMC.
This activity will greatly improve the predictive power of the simulations for modeling NQEs and provide in the longer term reliable methods that will generate synergies with several experimental groups working on kinetic isotopic effects, materials under high pressure, hydrogen transport in solids or on surfaces, which usually takes place by hopping through barriers, either via tunneling or thermal activation.

The Pierre et Marie Curie – Sorbonne University, at the heart of the Latin Quarter in Paris, is among the major scientific and academic institutions in France and shows a large panel of research activities, both experimental and theoretical. The research themes are part of a relatively young field with many new ideas coming up: active international collaborations are being set up to coordinate various strengths. The post-doc will actively take part in this process.

This post-doc is funded by Laboratory of excellence (Labex) MATISSE, with a net salary around 2300 € per month. As the post-doctorate should start before October 1st 2017, applicants are encouraged to contact us as soon as possible. Applicants should hold a Ph.D degree in Solid State Physics or Materials Science or Theoretical Chemistry, with expertise/experience in statistical mechanics and molecular dynamics, as well as programming languages. Knowledge and use of Density Functional Theory and/or Path Integrals are considered as a plus. Applicants should provide a CV with a list of publications and two references.

Scientific contacts:
Simon Huppert, huppert@insp.jussieu.fr, +336 72 81 50 76
Fabio Finocchi, fabio.finocchi@upmc.fr, +336 30 83 97 97
Administration (Labex MATISSE):
Laurence Bonnet-Lericque, laurence.bonnet-lericque@upmc.fr

References:

[1] Y. Bronstein, P. Depondt, L.E. Bove, R. Gaal, A.M. Saitta, et F. Finocchi, Phys. Rev. B 93, 024104 (2016).
[2] F. Brieuc, Y. Bronstein, H. Dammak, P. Depondt, F. Finocchi, M. Hayoun, J. Chem. Theory Comput. 12, 5688 (2016).
[3] S. Bonella, S. Meloni et G. Ciccotti, Eur. Phys. J. B, 85-97 (2012).
[4] A. Poma, M. Monteferrante, S. Bonella et G. Ciccotti, Phys. Chem. Chem. Phys. 14, 15458 (2012).