

PhD position at the Laboratory of Computational Science and Modelling, EPFL

A position for a fully-funded four-years doctoral program is available at the Laboratory of Computational Science and Modelling at EPFL, starting from May 2016, within the framework of the ERC Starting Grant project "HBMAP".

The project aims at unraveling the relations between molecular-scale building blocks and the emergence of meso-scale complexity, by using machine-learning analysis of state-of-the-art atomistic simulations. Novel, data-driven algorithms will be developed, implemented, and applied to predict and rationalize the behavior of materials and molecules, with a particular emphasis on hydrogen-bonded systems.

The applicant should have a Master or equivalent degree in a related subject, ability to speak and write effectively in English, be creative, independent and a good team player. Previous experience with atomistic modelling, some familiarity with a Unix/Linux environment and scientific programming (e.g. C++, FORTRAN or Python), and an interest in following the development of simulation techniques from the blackboard to the application to challenging materials problems. Previous experience with molecular dynamics, enhanced-sampling techniques and/or machine-learning strategies would be a plus, as well as first-hand knowledge of more general applications of machine-learning.

EPFL provides a thriving, international, English-speaking working environment with a strong inter-departmental expertise in computational materials modelling. It offers very attractive employment conditions, with a highly-competitive PhD salary. Candidates are encouraged to also apply to the EDMX doctoral school (<http://phd.epfl.ch/EDMX>). Admission is a requirement to be enrolled in the program.

A first round of applications will be evaluated by January 31st 2016. Please follow the instructions on <http://goo.gl/zQNHvy> when preparing your application.