1 PhD Position on Machine-learning Modeling for Nanoconfined Aqueous Systems

Join a European doctoral network involving some of the leading research groups on atomistic materials modeling, for an exciting doctoral project involving the study of water in confinement at the nanoscale, with relevant applications to catalysis, separation, and biophysics. The position is fully funded for the typical duration of a PhD (4 years, with a contract renewed yearly) with an attractive salary and great opportunities for training. The research topic focuses on the development of an integrated, physically-inspired machine-learning framework to drive simulations of these systems, including long-range effects and the interaction with external fields. An analogous position will be advertised at CECAM in the team of Dr. Sara Bonella, providing further opportunities for collaboration. Applicants are invited to send a one-page cover letter, a full CV including an extract of their exam results and contact information of two references to michele.ceriotti@epfl.ch, using "HIRING FLUXIONIC" as subject line. Evaluation of candidates will start immediately, and continue until the position is filled.

The MSCA-DN FLUXIONIC
FLUXIONIC is European doctoral network (MSCA-DN) focusing on controlled transport of matter in confined nano environments. At these scales, the macroscopic description of transport phenomena breaks down, and it is necessary to integrate experiments with fully atomistic model calculations and control non-equilibrium dynamics. Deeper understanding of these phenomena will foster technological developments and have an impact on core challenges for modern society: clean water, disease treatment, sustainable energy production/storage/usage.

FLUXIONIC gathers leading experimental and computational researchers from Spain, France, Denmark, Norway, the United Kingdom, and Switzerland. This team operates the intersection of Physics, Chemistry and Materials science and includes industrial researchers.

Machine-learning for nanoconfined water
This doctoral thesis will focus on the extension of state-of-the-art data-driven surrogate models of quantum mechanical calculations (including both machine-learning potentials, and models of dielectric response properties that are needed to estimate experimental observables) to incorporate the physical effects that are essential do describe aqueous systems in a confined environment. This includes for instance the description of long-range physical interactions, including static and polarizable electrostatics. Applications will include water confined in nanostructured silica, as well as potentially model systems relevant for biophysical processes.

Your profile
We are looking for a motivated student who is either recently graduated or about to receive their master / 4-year bachelor degree in chemistry, physics, materials science or computer science. Excellent analytical skills and an inclination for interdisciplinary research are a must, as well as a developed physical-chemical intuition. Familiarity with scientific programming, and experience with atomistic modeling and/or scientific machine-learning are important assets.

Your workplace
As an EPFL employee, you will be working in an international environment. We value the diversity of our team and particularly encourage women candidates to apply. In line with our values, EPFL encourages an inclusive culture. We promote equality of opportunity, value diversity and nurture a working and learning environment in which the rights and dignity of all our staff and students are respected. As a doctoral student you will receive an attractive salary complete with social security contributions, access to state-of-the-art computing facilities and to advanced training opportunities.