

1 PhD Position on Non-equilibrium Simulations of Ionic Transport in Confined Environments

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 ionic transport in confinement at the nanoscale, with relevant applications to batteries and supercapacitors. 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 non-equilibrium molecular dynamics for charged systems in external fields. An analogous position will be advertised at the COSMO Lab in the team of Prof. Michele Ceriotti, 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 sara.bonella@epfl.ch, using "HIRING FLUXIONIC" as subject line. Evaluation of candidates will start immediately, and continue until the position is filled.

Non-equilibrium Molecular Dynamics for Confined Charged Transport

This doctoral thesis will focus on the extension of state-of-the-art approaches to simulate the dynamics of charged systems in external electric and magnetic fields. Recently developed algorithms for studying nontrivial properties such as the ionic Hall effect in bulk will be adapted to simulations in confined environment. Implementations will study the behaviour of superionic water in supercapacitors and efficient and accurate inclusion of polarization effects in electrodes and electrolytes, with potential applications towards greener technologies.

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 physics, chemistry, or materials 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 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.

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.