

PhD position on molecular simulations applied to batteries shared by the PSA Group, ENS-Lyon and IFP Energies nouvelles

At the PSA group, a 3-year PhD position is available that makes part of collaboration between Ecole Nationale Supérieure de Lyon and IFP Energies nouvelles. The PhD is expected to start late summer or autumn 2019.

Subject: *the need for electrical energy storage becomes increasingly important both for transport applications and static large-scale flux batteries. Here we aim to develop a methodology based on atomistic simulations that in the end will help to screen electrolyte components in flux batteries or improve the understanding of electrochemical reactions involved in the aging of batteries.*

Theoretical Methods: *periodic DFT calculations and classical molecular dynamics simulations using a reactive force field.*

Complementary Information: *the PhD candidate will be hired by the PSA Group. The candidate will be trained at the Laboratoire de Chimie (ENS-Lyon) for specific DFT calculations that take into account electrically charged electrodes and at the Thermodynamics and Molecular Modeling Department of IFPEN for the reactive force field simulations. Additionally, the candidate will closely collaborate with the Department of Materials and Electrochemistry of IFPEN and the PSA Group.*

Mandatory expertise to apply: *eligible PhD candidates must have a solid background in theoretical/computational chemistry or physics and preferably also in molecular simulations.*

Remuneration: *we offer competitive salary and an attractive working environment in the region of Lyon and Paris (France).*

Contact: *for further information or applications, please contact Carine Michel (carine.michel@ens-lyon.fr), Theo de Bruin (theodorus.de-bruin@ifpen.fr) or Gentien Thorner (gentien.thorner@mpsa.com) with a detailed CV, a letter of motivation, 2 recommendation letters and a detailed academic record.*