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 Normale Supérieure de Lyon and IFP Energies nouvelles. This PhD is expected to start late summer or autumn 2020.

Background: *In the light of sustainable mobility, batteries play an essential role in the electrification and hybridization of transport vehicles. Batteries based on lithium ions currently offers one of the best performances with respect to other rechargeable batteries. However, in lithium ions batteries solid electrolyte interphase (SEI) layers are formed that can severely impact the performance of these batteries if they use graphite-based electrodes. Although, the origin of the formation of these SEI is now well-known, the factors that precisely control its formation, growth, passivating, transport and mechanical properties remain a subject of discussion in the literature.*

Project*: In this open PhD position we would like to shed more light on the formation and growth of those SEI layers using molecular modeling tools. More precisely, accurate periodic DFT calculations will be performed to optimize parameters that are used in an empiric reactive force field method. The latter allows us to simulate larger systems and at longer time scale than that can be performed using DFT. Both methods will be used to create a library containing the most essential elementary reactions with their kinetic rate constants. Such library will in turn be used to perform kinetic Monte Carlo (kMC) simulations to even further extend the time scale up to seconds.*

Theoretical methods: *periodic DFT calculations, classical molecular dynamic simulations using a reactive force field and kMC calculations**.***

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 a competitive salary and an attractive working environment in the region of Lyon and Paris (France).*

Contact: *for further information or applications, please contact Stephan Steinmann (stephan.steinmann at ens-lyon.fr), Theo de Bruin (theodorus.de-bruin at ifpen.fr), Carlos Nieto carlos.nieto at ifp.fr or Gentien Thorner (gentien.thorner at mpsa.com) with a detailed CV, a letter of motivation, 2 recommendation letters and a detailed academic record*.