PhD position at IFP Energies nouvelles (IFPEN)
In *Chemical science and Chemoinformatics*

Machine learning to optimize ReaxFF parameters

Computer simulation tools are widely used at IFP (Energies nouvelles (IFPen) for applications in various fields of energy, transport and the environment. The use of multi-scale modeling has become a key factor for successful studies. In chemistry, molecular modeling contributes to the understanding of phenomena occurring from electronic to mesoscopic scales. The explicit consideration of chemical reactions in molecular simulations requires the use of a so-called "reactive" force field such as ReaxFF. At IFPen, several studies involve the use of the ReaxFF force field with applications such as the corrosion of steels, the kinetics of soot oxidation... A challenging task with the application of ReaxFF still lies in the optimization of its parameters for a given system.

In recent years, we have applied various machine learning techniques, mainly to derive predictive models. Indeed, learning algorithms are very powerful tools for solving regression and optimization problems. The main objective of the proposed thesis subject stands in the development of an innovative approach to optimize parameters of the ReaxFF force field by application of learning algorithms. The proposed work is a joint PhD position between IFPen/UGent/SCM. It will be performed at the Ghent University, in close collaboration with research groups at IFPen and SCM. An opportunity to integrate the new features in the Amsterdam Modeling Suite program is possible after the PhD.

Keywords: Molecular simulation, ReaxFF, Machine learning

Academic supervisor	Prof. Dr. ir., VERSTRAELEN Toon, Center for Molecular Modeling, Ghent University (UGent), ORCID: 0000-0001-9288-5608.
Doctoral School	Doctoral School of Natural Sciences https://www.ugent.be/doctoralschools/en
IFPEN supervisor	Dr., CRETON Benoit, Research engineer, Thermodynamics and Molecular Simulation, benoit.creton@ifpen.fr
PhD location	Center for Molecular Modeling, Ghent University, Tech Lane Ghent Science Park, Campus Ardoyen, Technologiepark 46, 9052 Zwijnaarde, Belgium.
Duration and start date	3 years, starting not earlier than October 2020.
Employer	IFP Energies nouvelles, Rueil-Malmaison, France.
Academic requirements	University Master degree in physical or chemical science.
Language requirements	Fluency in English, and in French or willingness to learn French.
Other requirements	Knowledge in molecular simulation and/or machine learning techniques is mandatory.

For more information or to submit an application, see theses.ifpen.fr or contact IFPEN supervisors: benoit.creton(@)ifpen.fr and theodorus.de-bruin(@)ifpen.fr.

About IFP Energies nouvelles

IFP Energies nouvelles is a French public-sector research, innovation and training center. Its mission is to develop efficient, economical, clean and sustainable technologies in the fields of energy, transport and the environment. For more information, see https://www.ifpen.com.

IFPEN offers a stimulating research environment, with access to first in class laboratory infrastructures and computing facilities. IFPEN offers competitive salary and benefits packages. All PhD students have access to dedicated seminars and training sessions.