SUJET DE THESE / PhD SUBJECT

Tracking the degradation of organic compounds from reactive molecular dynamics simulations

The current project concerns the investigation of the chemical reactivity using molecular dynamics simulations and focuses on the degradation processes of pollutants. In this scope, the main objective of this PhD project is to enforce reactive molecular simulations applied to the degradation processes of organic compounds by considering both the thermodynamic and kinetic aspects of the reactivity. To that ends, the candidate will develop new methods in order to obtain reliable reactive FF for the considered compounds and improve the ReaxFF model itself.

Mots clés (Keywords): Molecular modelling, environment, molecular dynamics simulations, ReaxFF,

CONDITIONS D’EXERCICE / WORKING CONDITIONS

Laboratoire : IPREM
Site web : https://iprem.univ-pau.fr

Directeur de thèse (PhD Director): Germain Salvato Vallverdu
Co-Directeur de thèse (PhD co-Director):
En collaboration avec (In Collaboration with – if any)

Lieu (Place) : Pau, France

Date début (start): 01/10/2019  Durée (duration): 3 ans (years)

Employeur (employer): Université de Pau et des Pays de l’Adour (UPPA)

Salaire mensuel brut (monthly salary before taxes): 1768 €

SAVOIR-FAIRE DU LABORATOIRE / HOST LABORATORY PROFILE

The Institute of Analytical Sciences and Physico-Chemistry for Environment and Materials (IPREM) is a joint research unit CNRS / UPPA (UMR 5254). IPREM members are interested in the development of fundamental knowledge in physico-chemistry, analytical chemistry and microbiology, in relation to applications concerning the structure of the living, the management of the environment and the functional properties of different classes of materials. Their skills are based on analytical strategies, experimental and theoretical chemical-physics approaches, fine studies of structures and reactivity, development, characterization and implementation at different scales.

The skills of IPREM members in physical and theoretical chemistry concern the development of computational strategies at different time and space scales for the investigation of complex systems. These skills rely on a strong experience in various methodologies from quantum chemistry to classical molecular dynamics simulations.
MISSION - ACTIVITES PRINCIPALES / MISSION – PRINCIPAL ACTIVITIES

I. Le contexte scientifique / Scientific Context
Contamination of surface and groundwater with organic compounds (pharmaceutics compounds, pesticides ...) is a major concern due to the hazards these chemicals pose to the environment and humans. Depending on their aqueous solubility, the chemicals either remain in the soil or enter surface waters and groundwaters. The products that result from their degradation can remain in animals, vegetables and water sources, and are gradually enriched through the food chain. Because of the toxicity of certain compounds, even at trace levels, there is increasing interest in the development of systems to monitor, break down, and/or remove them.

II. Les objectifs / Objectives
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III. Plan de travail / Work plan
First of all, in order to investigate the degradation mechanisms of pesticides and chemicals, the ReaxFF parameters set has to be extended. To that ends, a training set containing conformers and reactive paths of the relevant compounds and their degradation products has to be built and target properties will be computed using quantum mechanical techniques. This quite difficult task will be tackled down by combining global optimizers that had been adapted to ReaxFF parameterization and homemade codes for the production and extraction of data from quantum chemistry calculations.
This will be achieved by the validation of the FF against experimental results. In particular, the coupling between molecular simulations and analytical chemistry experiments conducted using the high level instrumental facilities available in the IPREM institute will be implemented. At then end, you will consider the development of a robust and general procedure for the parameterization of ReaxFF.

IV. Références bibliographiques (Literature References)

Modifié le 02/10/2018
COMPETENCES REQUISES / REQUIRED COMPETENCES

The candidates must have knowledge in

- Physical chemistry and numerical simulation. Experience in molecular dynamics will be appreciated.
- Be proficient in numerical tools: Linux/Unix console, HPC server. Programming skills will be appreciated.

The candidates must demonstrate

- a good organization
- ability to present results issued from its research
- ability to work in a multidisciplinary team and to be capable of caring himself

CRITÈRES D’ÉVALUATION DE LA CANDIDATURE / CRITERIA USED TO SELECT CANDIDATE

Selection process steps:
- Establishment of the selection committee
- evaluation of the applicants cv’s
- Interview with the selected candidates and ranking.
Criteria used in selection of the candidate:
- The candidate’s motivation, scientific maturity and curiosity
- Adequation between candidate skills and the Phd project
- English proficiency

CONSTITUTION DU DOSSIER DE CANDIDATURE / REQUIRED DOSSIER,

send an e-mail with your candidature containing :

- CV
- cover letter detailing candidate’s motivations
- candidate’s MSc marks and ranking
- any letters of recommendation
- minimum two contact details for 2 referees

DATE LIMITE DE DEPOT DU DOSSIER (limiting date): 05/07/2019

CONTACTS

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