Polytech network form for PhD Research Grants from the China Scholarship Council

This document describes the PhD subject and supervisor proposed by the French Polytech network of 14 university engineering schools. Please contact the PhD supervisor by email or Skype for further information regarding your application.

Supervisor information	
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PhD information	
Title	Multiscale molecular dynamics simulation of persistent organic pollutant abatment: from fundamentals to efficient processing
Main topics regards to CSC list (3 topics at maximum)	I.1 ; V-12 ; VI-3

Required skills in science and engineering	Molecular dynamics simulation, physics and chemistry of reactivity, plasma chemistry and physics

Subject description (two pages maximum)

Abatment of water and soil pollutions is a major challenges for the next century. Progress in agriculture and health care have generated a large set of persistant organic pollutants (POPs) targeting culture protection against insects and wild plants that hamper efficient food primary agricultural production efficiency. But, it becomes clear now that some kind of these persistent oganic molecules are recognized as being disease agents, especially endocrine disruptors and/or carcinogenic.
Among all them [1-3], organo-chlorine (Polychlorinated biphenyl, atrazine, ..), -phosphate (glyphosate, …) are deserving special attention as they are persistently present in soil and water. Recently, chlordecone has been subjected to a special attention in France to its high level in Caribbean French islands.

As new programs are build around the world for limiting and suppressing use of these herbicides and insecticides, it is necessary, in the mean time, to remove existing pollutants in the environment.

The present project, will deal with understanding which are the advanced oxidation path of selected molecules as glyphosate, atrazine and polychlorinated biphenyl.

Actually tehermochemicals treatments of such molecules adsorbed on activated carbons are the preferred ways of destruction. An emerging technique is the non-thermal plasma treatment of contaminated water. In both cases, a fundamental question arises : what are the reaction products and are they less toxic than the parent molecules.

For answering such a crucial question, the present project will propose to carry out mulsticale molecular dynamics simulations of the advanced oxidation of these molecules in conditions matching the experiments.

The relevance of such simulations will be ensured by using reactive force fields that allow to properly take into account bond breaking/formation of radicals [4].

The output of the simulation will be the reaction paths towards products [5] and thus it will be possible to determine all the energetic barriers and thus find which is the best chemical engineering process for removing/destroying the toxic molecules. Moreover, adding explicitly electric fields in the simulations will give opportunity to evaluate the potential of plasma chemical processing for solving such an issue.

The candidate will have acces to supercomputing facilties appropriate for his/her simulations.

References

[1] Stockholm Convention on Persitent Organic Pollutants (2009 amendments)
[2] State of the Science of Endocrine Disrupting Chemicals, Edited by Åke Bergman, Jerrold J. Heindel, Susan Jobling, Karen A. Kidd and R. Thomas Zoeller, INTER-ORGANIZATION PROGRAMME FOR THE SOUND MANAGEMENT OF CHEMICALS, A cooperative agreement among FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank and OECD
[3] IARC monographs on the evaluation f carcinogenic risks to humans, some organophosphates insecticides and herbicides, Vol. 112, International Agency of Research on Cancer-WHO
[4] TP Sentfle et al, The ReaxFF reactive force-field: development, applications and future directions, npj Computational Materials (2016) 1501
[5] K Chenoweth, ACT van Duin, WA Goddard, IIIReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation, J. Phys. Chem. A, 2008, 112 (5), pp 1040–1053