CollaMASTER DE PHYSIQUE - 2ème année
Physics of Complex Systems

Proposition de stage 2018-2019

Laboratoire: Laboratoire de Chimie Théorique, Sorbonne Université **Adresse:4, Place Jussieu, 75005 Paris** **Directeur du laboratoire: O. Parisel (J.-P. Piquemal du 01/01/2019)**	
Responsable(s) du stage: Riccardo Spezia **Téléphone: 01 44 27 70 87** **e-mail:riccardo.spezia@sorbonne-universite.fr**	**Collaboration :CentraleSupélec SPMS** **Hichem Dammak** **hichem.dammak@centralesupelec.fr**

Titre du sujet proposé
Introducing Vibrational Quantum Effects in Reaction Dynamics Simulations

***Projet scientifique* :**
The aim of the project is to include vibrational quantum effects in Born-Oppenheimer molecular dynamics simulations to model and understand chemical reactivity. At this end, new advances in the field of computational physics will be used to improve the dynamical description of chemical reactions.
Thanks to developments in electronic structure theory, it was possible to study gas phase reactivity of relatively large molecules, like carbohydrates and poly-peptides [1]. The next step is to improve the physical description of chemical reactions by adding nuclear quantum effects.
Recently, Dammak and co-workers have developed a method called Quantum Thermal Bath (QTB) which introduces vibrational quantum effects at virtually no additional computer cost [2]. This method is based on Langevin-like equations of motion with a colored random noise. The implementation of this method in the reaction dynamics code VENUS was done recently and it can now be tested and eventually improved.
As test case, unimolecular fragmentation models and reactions of astrophysical interest will be considered [3].

[1] K.Song and R.Spezia. *Theoretical Mass Spectrometry.* De Gruyter, Berlin (2018).
[2] H.Dammak, Y.Chalopin, M.Laroche, M.Hayoun and J.-J.Greffet. *Phys. Rev. Lett.* 103, 190601 (2009).
[3] R.Spezia, J.-Y.Salpin, M.-P.Gaigeot, W.L.Hase and K.Song. *J. Phys. Chem. A* 113, 13853–13862 (2009); R.Spezia, Y.Jeanvoine, W.L.Hase, K.Song and A.Largo. *Astroph. J.* 826, 107 (2016).

Techniques utilisées : molecular dynamics simulations, quantum thermal bath

Qualités du candidat requises : use of Linux environment and basis of informatic coding

Rémunération éventuelle du stage : oui
Possibilité de poursuivre en thèse ? oui
Si oui, mode de financement envisagé : possible un financement Sorbonne Université

Ne pas dépasser une page, svp.