MASTER DE CHIMIE DE PARIS CENTRE - M2S2

Proposition de stage 2022-2023

Internship Proposal 2022-2023

Parcours type(s) / *Specialty(ies) :*

X Chimie Analytique, Physique et Théorique */ Analytical, Physical and Theoretical Chemistry* :

☐ Chimie Moléculaire / *Molecular Chemistry* :

☐ Chimie et Sciences Du Vivant / *Chemistry and Life Sciences* :

☐ Chimie des Matériaux / *Materials Chemistry:*

☐ Ingénierie Chimique / *Chemical Engineering:*

Laboratoire d'accueil / *Host Institution*

Intitulés / *Name* : Laboratoire de Chimie Théorique, Sorbonne Université

Adresse / *Address* : 4, place Jussieu, 75005 Paris

Directeur / *Director (legal representative) : Jean-Philip Piquemal*

Tél / *Tel* :

E-mail : Jean-Philip.Piquemal@sorbonne-universite.fr

Equipe d'accueil / *Hosting Team : Méthodologie*

Adresse / *Address :* 4, place Jussieu, 75005 Paris

Responsable équipe / *Team leader* : Julien Toulouse

Site Web / *Web site :*

Responsable du stage (encadrant) / *Direct Supervisor : Peter Reinhardt*

Fonction / *Position :Maître de Conférences (HDR)*

Tél / *Tel* : 01 44 27 96 57

E-mail : Peter.Reinhardt@sorbonne-universite.fr

Période de stage / *Internship period* [1] : février – juin 2023

1* min. 5 mois à partir du 30 janv 2023 / *min. 5 months not earlier than January, 30st 2023.*
Fin de stage au plus tard le 13/07/2023 ou le 29/09/2023 (dates de validation de diplôme). / *End of internship at the latest July 13, 2023 or Sept. 29, 2023 (dates of graduation).*

Potential surface and simulation of isotope exchanges for the gas-phase reaction CO + O → CO_2 → CO + O

Projet scientifique (1 page maximum) / ***Scientific Project (maximum 1 page):***

1. Description du projet / *Description of the project*

Isotope exchanges are an interesting object for studying quantum effects on atomic or molecular systems. The puzzling case of the ozone anomaly has been studied since its discovery 40 years ago. A similar case is that of the carbon monoxide oxidation, with the supplementary difficulty of a spin change during collision between the fragments CO + O (triplet) and the reaction product CO_2 (singlet).

The first ingredient for a simulation with molecular dynamics is a potential surface. Based on previous work the proposed internship aims at completing the data towards a usable, smooth set with an asymptotic continuation for the first states of the potential surface. Once this surface available, classical molecular dynamics sampling the possible different initial conditions can be conducted in order to extract a mass-independent isotope fractionation as obtained for ozone.
Beside notions of multi-reference ab-initio calculations (MCSCF, MRCI) programming skills (Linux, python, …) will be helpful.

The proposed interrnship is part of the ANR project « MIF – mass-independent fractionation » in collaboration with the MNHN, the IPGP and Sorbonne Nord (Villetaneuse).

2. Techniques ou méthodes utilisées / *Specific techniques or methods*

Ab-initio multi-reference calculations, spline interpolation, extrapolation, non-linear multi-dimensional data fitting, visualization with gnuplot or Mathematica

3. Références / *References*

F Robert, P Reinhardt, « Mass independent isotopic fractionation: A key to plasma chemistry », Chemical Physics Impact **4** (2022) 100073 (https://doi.org/10.1016/j.chphi.2022.100073)