**MASTER DE CHIMIE DE PARIS CENTRE - M2S2**
**Proposition de stage 2021-2022**
**Internship Proposal 2021-2022**

**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, LCT UMR 7616
Adresse / *Address* : Sorbonne Université, 4 Place Jussieu, 75005 Paris
Directeur / *Director (legal representative) :* Jean-Philip PIQUEMAL
Tél / *Tel* : 01 44 27 25 04
E-mail : jean-philip.piquemal@sorbonne-universite.fr

**Equipe d'accueil / *Hosting Team :* Dynamics Simulations : Structure and Reactivity**

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Fonction / *Position :* Directeur de Recherche CNRS & Maitre de Conférence
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Période de stage / *Internship period* * : fevrier-juillet 2022

***** min. 5 mois à partir du 31 janv 2022 / *min. 5 months not earlier than January, 31st 2022.*
Fin de stage au plus tard le 15/07/2022 ou le 30/09/2022 (dates de validation de diplôme). / *End of internship at the latest July 15, 2022 or Sept. 30, 2022 (dates of graduation).*

**Titre / *Title***

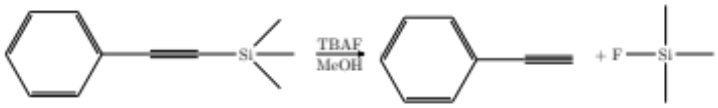
# Modeling Reaction Kinetics Modified by Vibrational Strong Coupling

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

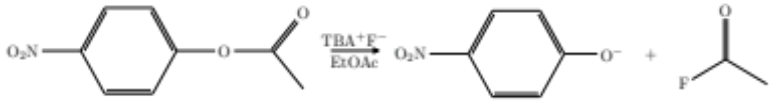
1. Description du projet / *Description of the project*

Recently, it was shown that chemical reactivity can be modified when performed into a micro-cavity which is in resonance with (at least) one vibrational mode[1].
The field of vibrational strong coupling (VSC) is now the topic of a growing interest from both experimental and theoretical sides, but a clear picture and rationale of the process are still missing.

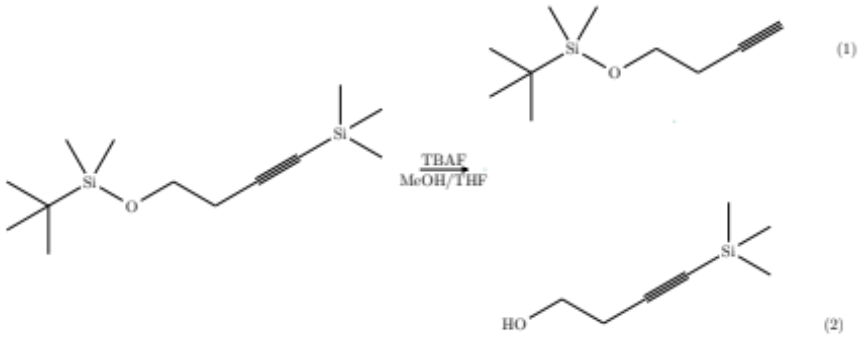
The aim of the project is to describe the reactions for which the kinetics is modified by the VSC, as particularly by Ebbesen and co-workers.
In particular, we propose to focus the attention first on the following reactions :
a) SN2 reaction [2,3]




b) bond breaking with formation of an ionic product [4]




c) competition between two reaction pathways [3,5]




This internship is part of an ANR project started in January 2021 on modeling and manipulating vibrational strong coupling, with the aim of understanding the effect of the coupling on the chemical reactivity as it was recently shown [1]. The team is composed by two theoretical chemistry groups (at Sorbonne Université and at ENS Paris) and the micro-fluidic group at ENS.

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

During the internship, the student will first use different methods of quantum chemistry to understand the reaction profiles in the most accurate way. A first realistic model will be using density functional theory (DFT) with an implicit solvent. This part will be also useful to have a reference for further use of less expensive methods, like tight-binding DFT, semi-empirical Hamiltonians and possibly reactive force fields. These last methods, in fact, are likely to be used in reaction dynamics simulations.

3. Références / *References*

1) J.A.Hutchison, T.Schwartz, C.Genet, E.Devaux, T.W.Ebbesen. Angew. Chem. Int. Ed. **2012**, 51, 1592 ; A.Shalabney, J.George, J.Hutchison, G.Pupillo, C.Genet, T.W.Ebbesen. Nature Comm. **2015**, 6, 5981.
2) A.Thomas, et al. Angew. Chem. Int. Ed. **2016**, 55, 11462.
3) C.Climent and J.Feist. Phys. Chem. Chem. Phys. **2020**, 22, 23545.
4) J.Lather, P.Bhatt, A.Thomas, T.W.Ebbesen, J.George. Angew. Chem. Int. Ed. **2019**, 58, 10635.
5) A.Thomas, et al. Science **2019**, 363, 615.