



M2 Internship

TITRE	Charge, Energy transfer and chemical Reaction with molecules in an electromag- netic Cavity	
LABORATOIRE	Laboratoire Ondes et Matière d'Aquitaine (LOMA), CNRS and Univ. Bordeaux	
RESPONSABLE(S)	Rémi Avriller. <u>https://www.loma.cnrs.fr/remi-avriller/</u> Team <u>https://www.loma.cnrs.fr/thematique-quatems/</u>	
CONTACT		
Téléphone		e-mail
05 40 00 89 56		<u>remi.avriller@u-bordeaux.f</u> r

Project

Context. Recent progresses in nanotechnology led to the creation of a new generation of nano-structures playing the role of electromagnetic cavities, like plasmonic structures [1] (see Fig.1), organic micro-cavities [2] and nano-fluidic Fabry-Pérot cavities [3]. The first experimental proof of reaching the *electronic strong-coupling regime* for cavity-confined molecular populations was reported recently [2,3]. The confinement has important consequences on the physico-chemical properties of the confined molecules, with remarkable effects on the kinetics of chemical reactions [2].



Adapted from [1].

In this M2 internship, we propose to investigate original and innovative nano-probes and open chemical nano-reactors in order with a single-molecule embedded inside. to *initiate*, *probe* and *modulate* the rate of chemical reactions at the nanoscale.

We will propose from the point of view of theory, alternative ways of building open chemical reactors using state-of-the-art nanotechnology. Two relevant cases for chemistry will be investigated: (i) passing an electronic current across the tip of an STM plasmonic hot-spot involving single molecules, (ii) using a stationary flow of reactants in solution, entering and leaving an open-chemical reactor made of a nano-fluidic optical cavity. We will identify crucial physical ingredients related to the strong-coupling between *electronic* or vibrational degrees of freedom of the embedded molecules and a cavity photon mode (cavity-polaritons), and incorporate them into the description of chemical reactions.

The scientific environment and collaborators. The candidate will benefit from an international and dynamic scientific environment within the Transborder Joint Laboratory (LTC), Theoretical Chemistry and Physics at the Quantum Scale (http://www.quantumchemphys.org/), involving the Universities of Bordeaux (France), Basque Country (UPV/EHU, Spain) and the Donostia International Physics Center (DIPC, Spain).

The candidate profile. The candidate should have a strong background in one of the following disciplines: quantum physics, quantum optics, condensed matter, theoretical physics or chemistry, statistical physics. Good skills in analytical methods, scientific computing and English would be appreciated. A PhD fellowship will be financed by the Agence Nationale de la Recherche, project CERCa.

- **References:** [1] R. Chikkaraddy et al., Nature **535**, 127 (2016).
 - [2] J. A. Hutchison et al., Angew. Chem. Int. Ed. 51, 1592 (2012).
 - [3] H. Bahsoun, et al., ACS Photonics 5, 225 (2018).

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