Post-doctoral fellowship (2 years) in Theoretical Chemistry

Modeling Reaction Kinetics Modified by Vibrational Strong Coupling

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 [2].

At this aim we will couple reactive molecular dynamics (likely using the CP2K software) with the cavity Born Oppenheimer scheme [3]. This will be extended including the path integral based development currently performed in the group. A first issue will focus on spectroscopic signatures, which is characterized by a Rabi splitting on the reactant and/or solvent molecules vibrational spectra in presence of VSC. The reaction free energy will then be obtained in presence and absence of VSC. DFT and/or DFTB methods will be investigated to address these reactions with methods which have a good balance between reliability and computational efficiency.

This fellowship is part of an ANR project started in January 2021. The team is composed by two theoretical chemistry groups (at Sorbonne Université and at ENS Paris) and the micro-fluidic group at ENS.

The candidate must have a PhD in theoretical chemistry, computational physics or related disciplines, with experience in *ab initio* molecular dynamics simulations (or equivalent approaches). The knowledge and experience in scientific programming is necessary.

Contact & Information

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References

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2) A.Thomas, et al. Angew. Chem. Int. Ed. **2016**, 55, 11462.; J.Lather, P.Bhatt, A.Thomas, T.W.Ebbesen, J.George. Angew. Chem. Int. Ed. **2019**, 58, 10635; A.Thomas, et al. Science **2019**, 363, 615; K.Nagarajan, A.Thomas, T.W. Ebbesen. J. Am. Chem. Soc. **2021**, 143, 41, 16877.
3) T.E. Li, J.E. Subotnik, A.Nitzan. Proc. Natl. Acad. Sci. USA **2020**, 117, 18324.