

PhD Studentship in Theoretical Chemistry

Nuclear Quantum Effects in Ion-molecule Reactivity via Molecular Dynamics Simulations

The aim of the project is to consider and study nuclear quantum effects (NQE) in Born-Oppenheimer molecular dynamics to address, in particular, ground-state reactivity with relevance to mass spectrometry and astrochemistry. We plan to use and implement Quantum Thermal Bath (QTB) and Ring Polymer Molecular Dynamics (RPMD) in the VENUS code which is interfaced with MOPAC and DFTB+. Two main NQEs will be relevant to these problems: zero-point energy leakage in unimolecular fragmentation and proton tunneling. An important part of the project will be to implement and optimize QTB and RPMD methods into VENUS considering the specificity of gas phase ion-molecule reactions. Examples of applications will be in the formation of complex organic molecules in gas phase induced by IR photons eventually also at solid/vacuum interface.

The candidate should have a Master (or equivalent) in Theoretical and/or Computational Chemistry or related atomistic/molecular sciences (Computational or Molecular Physics etc ...). The knowledge of scientific programming is required. Speaking French is not required.

The PhD will be done in *Sorbonne Université*, Science Faculty (downtown Paris, Latin quartier) in the *Laboratoire de Chimie Théorique* (www.lct.jussieu.fr), which is an internationally renewed laboratory in theoretical and computational chemistry.

The student will be supervised by Dr. Riccardo Spezia, which leads the group "Reaction Dynamics". Collaborations with both theoretical (at Physics Department) and experimental (at Université Paris-Saclay) groups are envisaged.

Candidates should contact the future PhD advisor, with a full CV and two contacts for references.

Dr. Riccardo Spezia, CNRS research director (research professor)

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Recent publications related to the project:

1.R.Spezia and H.Dammak. *On the Use of Quantum Thermal Bath in Unimolecular Fragmentation Simulation*. J. Phys. Chem. A **123**, 8542-8551 (2019).

2.D.Scuderi, A.F.Perez-Mellor, J.Lemaire, S.Indrajith, J.-X.Bardaud, A.Largo, Y.Jeanvoine and R.Spezia. *Infra-Red Assisted Synthesis of Prebiotic Glycine*. ChemPhysChem **21**, 503-509 (2020).