



PhD position in Paris starting in Fall 2018

Group of Guillaume Stirnemann, CNRS Institut de Biologie Physico-Chimique, Paris, France

Towards a molecular understanding of thermophoresis and its relevance for precursor accumulation in the context of life's origins

Subject In modern cells, molecules are confined in a volume in the femtoliter range, resulting in concentrations that critically enhance reaction rates. How can an efficient chemistry leading to the emergence of life take place in an ocean, a puddle or even a water droplet, which are 10^9 - 10^{36} times larger? Recent pioneer experiments have shown that thermally-driven processes such as thermophoresis can accumulate otherwise dilute precursors at localized spots acting as thermal traps for RNA strands oligomerization. Natural thermophoretic settings occur e.g. in the pores of hydrothermal vents on the ocean's floor that may have played a key role in the appearance of biological chemistry. On a different perspective, the number of technological applications that use thermophoresis is burgeoning, including the manipulation of biomolecules in thermal traps, the measurement of protein-ligand affinity or applications in microfluidics.

Yet, a major limitation is that the nature of thermophoresis is still highly debated. The goal of this PhD will be to use all-atom molecular dynamics simulations of *in silico* realizations of thermophoretic settings and analytical modeling to gain a deeper molecular understanding of this phenomenon. The PhD candidate will learn how to use distributed molecular dynamics packages for systems ranging from small ideal solutes up to biomolecules, how to use advanced accelerating techniques, how to extract relevant molecular information from the simulated trajectories, and how to implement additional simulation algorithms if required.

Research environment Research will take place in the group of Guillaume Stirnemann in the lab of Theoretical Biochemistry of the CNRS Institute of Physical and Chemical Biology (CNRS is the French national research agency). It is located in the very stimulating research environment of the Latin Quarter, at the heart of Paris. Our group has extensive experience in applying advanced simulation and theoretical tools to tackle a variety of questions, ranging from water ultrafast dynamics in aqueous solutions to the mechanical and thermal stability of proteins. We have access to state-of-the-art computing facilities that include a local mesoscale computer cluster. The PhD salary includes generous health and social benefits, and a number of housing opportunities are available for foreign applicants. Funding is provided for 3 years (with a possible extension if necessary) by the European Research Council (Starting Grant ABIOS). More information about the lab and the research group are available here: www-lbt.ibpc.fr/people/stirnemann.

Requirements Master degree or equivalent in molecular physics or physical/theoretical chemistry. A previous experience with simulations or programming would be an advantage but is not required.

Contact information Interested candidates should contact Guillaume Stirnemann as soon as possible (stirnemann@ibpc.fr), together with a curriculum vitae and contact information for one or two references.

