



PhD position in Paris starting in Fall 2018

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

RNA synthesis in abiotic conditions: addressing the challenge of phosphoester bond formation

Subject The idea that life would have evolved from RNA-based enzymatic systems preceding modern proteins – later coined as the “RNA World” hypothesis – has been considerably reinforced by the discovery that RNA, which can carry genetic information, is also capable of catalysis. An ultimate proof would be the experimental evidence for RNA synthesis and self-replication in abiotic conditions. But despite 70 years of intense research, the demonstration has not been achieved. In particular, the formation of phosphoester bonds between RNA nucleotides in abiotic conditions remains very challenging.

In order to enhance the reaction rate in abiotic conditions while improving its regioselectivity, a variety of more reactive intermediates and/or catalysts have been experimentally suggested, but the energetics of the reaction and the effect of such conditions are poorly understood at a theoretical level. The goal of this PhD will be to use ab-initio molecular dynamics as well as mixed quantum/classical approaches to gain a deeper molecular understanding of phosphoester bond formation, and to understand how plausible catalysts and activators can help enhance the rate and the regioselectivity of the reaction. The PhD candidate will learn how to use distributed classical and ab-initio molecular dynamics packages for systems, 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 lab of Theoretical Biochemistry of the CNRS Institute of Physical and Chemical Biology with Guillaume Stirnemann and Charles Robert. 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.



European
Research
Council