

Internship offered in M2 2018-2019

Responsible for internship

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Location : IMPMC - 4 place Jussieu,
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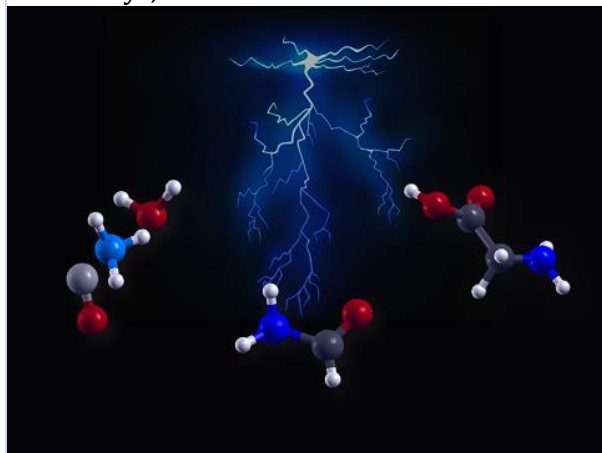
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Internship topic: *Role of phosphorus and minerals in the emergence of life*

Nowadays, there is a consensus on the fact that life might have emerged from the primordial soup



around 4 billion years ago, but little is known about the evolution of simple organic molecules into more and more complex biopolymers. In particular, the “RNA world” hypothesis states that today’s biology based on DNA and proteins may have been preceded by a primordial time where RNA would simultaneously play a (simplified) role of chemical synthesis and chemical information. However, even the emergence of the basic constituents of RNA, the nucleotides (formed by nucleobases, sugars and phosphate ions), is not understood yet. A fascinating hypothesis is that **clays** could be considered the inorganic prebiotic ancestors of biological molecules, as they can both carry information and catalyse their own synthesis (=reproduce). This

possibility has never been demonstrated, experimentally and/or by computer simulations.

In this master project, we propose to combine state-of-the-art *ab initio* calculations with top-notch experiments (done by the collaborators indicated above), to study the interaction of phosphate ions and clays, in the presence of the precursors of biomolecules. To this end, we will employ the advanced *ab initio* free-energy methods that we have developed in our team.

We look for a student strongly determined to undertake this ambitious and potentially breakthrough project, within a young and dynamical team. We have a consolidated expertise and a strong publication record in the development of advanced approaches, successfully applied to the study of molecular systems, including 7 PNAS, 2 Nature Comm and 8 PRL in the last few years. We have an ongoing prebiotic chemistry/origins of life collaboration with the NASA Goddard Center, and we have been recently invited to write a review article on computational approaches to origins of life studies in the most prestigious review of the field, Physics of Life Reviews <https://doi.org/10.1016/j.pprev.2018.09.004>

Techniques involved: Ab initio calculations, metadynamics, free-energy methods

Applicant skills: strong background in physical chemistry, propensity for simulations and/or programming

Paid internship: Yes

Can this internship be continued for a PhD? Yes

If yes, type of PhD funding envisaged is: Labex, Ministère, autres