2020-2021

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

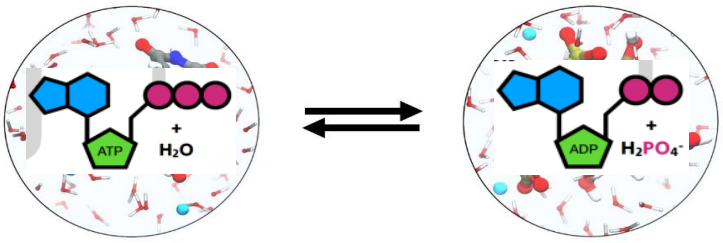
Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: Guillaume Fiquet

Title: ATP synthesis and origins of life studies from computational ab initio and machine learning methods

Keywords: ATP, prebiotic chemistry, origins of life, ab initio simulations, machine learning, phase space explorations

Scientific description:

Adenosine-triphosphate (ATP) is one of the most important biomolecules, as it is universally used by living entities as the main "generalist energy currency", to stock chemical energy, and then to be released to favor crucial biochemical reactions. However, it is not known yet "why" (i.e. with respect to many other chemical possibilities) and "how" (i.e. in which "prebiotic" conditions) this particular chemical species has been selected by nature.



Building on our recent breakthroughs in computational prebiotic chemistry, achieved thanks to state-of-the-art *ab initio* free-energy methods, we are strengthening our approaches through the in-house ongoing development of quantum accuracy-level machine learning potentials, capable to address challenges in the study of chemical reactions in more and more complex and realistic environments.

In this internship project, which will lead to a PhD thesis, we will study, at an unprecedented level of both accuracy and complexity, the crucial steps of ATP synthesis and degradation in both biological-like and prebiotic-like conditions, in order to achieve a full understanding, from the thermodynamic and kinetic point of view, of the synthesis of this universal chemical entity.

We look for a student willing to undertake these innovative methods and determined to carry out the project in connection with our network of collaborations with LNLL and NASA. We have a consolidated expertise and a strong publication record including, in the last few years, 7 PNAS, 5 PRL, 4 SciRep, 2 Nature Comm, 1 Nature Methods, 1 ChemSci, and 1 review in the field of origins of life research.

Techniques/methods in use: statistical analysis, *ab initio* molecular dynamics and free-energy methods, machine learning

Applicant skills: strong background in statistical physics, interest in computational materials science, basic knowledge in transformations in condensed matter physics and chemistry

Industrial partnership: N

Internship supervisor(s) (name, email, phone, webmail):
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Internship location: IMPMC – Campus Pierre et Marie Curie – T 2324

Possibility for a Doctoral thesis: Y (specific funding very likely, otherwise doctoral school)