Master 2: *International Centre for Fundamental Physics*
INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
CNRS identification code: UMR 7590
Internship director'surname: A. Marco SAITTA – PR
e-mail: marco.saitta@sorbonne-universite.fr Phone number: 0144275236
Internship codirector'surname: Rodolphe VUILLEUMIER – Dép Chimie ENS
Internship location: IMPMC – SU – Campus Pierre et Marie Curie
Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: PEPR/Labex/Idex, or ED's

Prebiotic chemistry/origins of life studies from computational ab initio and machine learning methods

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 the RNA nucleotide 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 will in particular develop and consolidate novel statistical physics methods for accurate predictions in kinetics, by using generalized Langevin equation approaches.

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, 8 PNAS, 5 PRL, 3 Nature Comm, 4 J Phys Chem Lett, 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 methods for condensed matter physics and chemistry, good knowledge in machine learning would be a plus.
Key words: theory, statistical mechanics, simulations, machine learning
The supervisor "in action":

Video from my Colloquium at the Physics Department of ENS

Condensed Matter Physics: YES Macroscopic Physics and complexity: YES
Quantum Physics: YES Theoretical Physics: YES