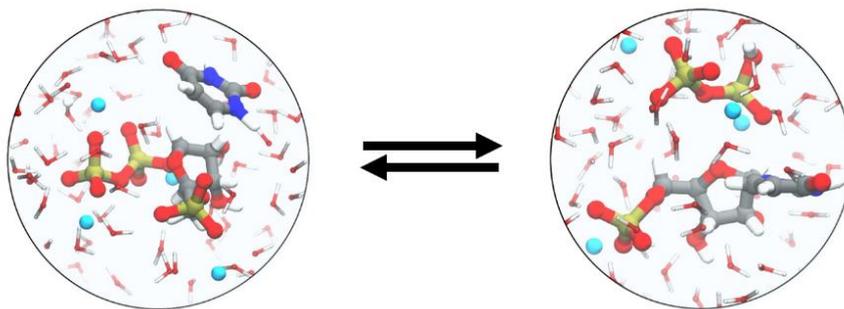


**Title:** Machine learning methods for computational studies in origins of life

**Keywords:** Machine learning, origins of life, ab initio simulations, phase space explorations

**Scientific description:**

Modern research in understanding the physical basis of the origins of life is becoming more and more quantitative, thus requiring the use of more and more advanced and sophisticated methods in computational physics and chemistry. Building on our recent breakthroughs in this field, achieved thanks to state-of-the-art *ab initio* free-energy methods, we aim to go further, and develop quantum accuracy-level machine learning potentials, capable to address challenges in the study of chemical reactions in more and more complex and realistic environments. We will exploit a theoretical collaboration with Lawrence Livermore National Labs, and an experimental one with NASA Goddard Space Center. Our results will advance our fundamental understanding of the main classes of prebiotic chemical reactions. In addition, the modeling of reactions in complex conditions will be done with general-purpose and flexible methods to allow the discovery of unknown chemical pathways.



We look for a student willing to develop these innovative methods and determined to carry out the project in connection with our network of collaborations. 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, clustering, local and global descriptors, *ab initio* molecular dynamics

**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):

A. Marco Saitta [marco.saitta@sorbonne-universite.fr](mailto:marco.saitta@sorbonne-universite.fr) 0144272244

Fabio Pietrucci [Fabio.pietrucci@sorbonne-universite.fr](mailto:Fabio.pietrucci@sorbonne-universite.fr) 0144275230

**Internship location:** IMPMC – Campus Pierre et Marie Curie – T 2324

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