Master 2: *International Centre for Fundamental Physics*

INTERNSHIP PROPOSAL

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Thesis possibility after internship: YES
Funding: Ecole Doctorale EDPIF

Reverse engineering of chemical reactions

Finding ways to accelerate chemical reactions or to increase the yield of rare products are widely studied problems in quantum or classical chemistry. If the chemical reaction is simple, solutions can be found by controlling and optimizing a small number of key parameters. However, this is untractable for more complex reactions and new strategies are needed.

One idea would be to make chemistry more programmable, in a way similar to electronic circuits. In order to do so, we need to understand the rules by which different chemical reactions can be associated and combined within «chemical programs» in order to achieve a given function despite fluctuations due to errors and noise. These rules should emerge from conservation laws and thermodynamic principles, and need to be tested on statistical physics models.

Another important aspect is to understand how information can be stored and processed by chemical networks. Taking inspiration from biological systems, we expect that robust and efficient chemical networks should appear as the result of a learning process of trials and errors similar to that of natural selection. To model such processes, we plan to use population dynamics, information theory and machine learning.

No specific knowledge in any of these fields are required; only basic knowledge of statistical physics and thermodynamics is expected. This project will benefit from close interactions with the experimental group of Y. Rondelez, «Systèmes et programmes moléculaires», which is also part of the Gulliver lab at ESPCI.

References:

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