INTERNSHIP PROPOSAL

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Thesis possibility after internship : YES
Funding: YES (ANR)

Statistical Physics of Catalysis

Catalysts, which accelerate chemical reactions without being changed in the process, are essential to life as much as to chemical engineering. The best known catalysts are enzymes, proteins from biological organisms that are not only extremely efficient but also capable of evolving through random mutations to catalyze new reactions. Understanding how enzymes achieve these feats is a long-standing problem where fundamental physical questions remain open [1].

We are currently developing a statistical physics approach to this problem, inspired by two lines of work:

(1) Theoretical work explaining another puzzling property of proteins, their ability to quickly fold into unique three-dimensional structures — the so-called protein folding problem. The underlying principles have been uncovered through a combination of physical models, numerical simulations and experiments [2]. We are taking a similar approach to understand the principles of catalysis [3].

(2) Recent experiments with programmable matter demonstrating the design and manipulation of micron-scale artificial "molecules" with interactions that can be tuned at will to mimic and study systematically properties displayed by biological systems [4]. Most of these experiments have so far focused on self-assembly, the formation of structures from collections of diverse building blocks [5]. A current PhD student in our group has shown computationally how catalysis could be introduced in these experiments, thus opening a new avenue to study catalysis through the lens of physics [6].

The internship will consist in the theoretical study of coarse-grained physical models of catalysis that we are currently developing. The goal will be to show how the catalytic principles that we previously identified in simple designs [3,6] can be implemented in this framework and then to extend our previous findings to study new principles with, in particular, applications to the design of autocatalysts, catalysts that accelerate their own formation.

The work will involve analytical calculations and numerical simulations of stochastic processes. A very good knowledge in statistical physics is required but no previous knowledge in catalysis is expected.

The internship will take place in the context of several collaborations with colleagues from different disciplines — physics, biology, chemistry — taking different approaches — theory, numerical simulations, evolutionary analyses, experiments — with a common interest in catalysis and its implications for our understanding of the nature and origin of life and the engineering of sustainable technologies.

References

[1] Agarwal, PK. A biophysical perspective on enzyme catalysis. *Biochemistry* 58 (2018): 438-449.

[2] Onuchic, JN, and PG Wolynes. Theory of protein folding. *Curr Op Struct Biol* 14 (2004): 70-75.

[3] Rivoire, O. Geometry and flexibility of optimal catalysts in a minimal elastic model. *J Phys Chem B* 124 (2020): 807-813.

[4] Jones, MR, NC Seeman, and CA Mirkin. Programmable materials and the nature of the DNA bond. *Science* 347 (2015): 1260901.

[5] Cademartiri, L, and KJM Bishop. Programmable self-assembly. *Nature materials* 14 (2015): 2-9.

[6] Munoz Basagoiti, M, O Rivoire, and Z Zeravcic, Catalysis from the bottom-up (in preparation)