Master 2: *International Centre for Fundamental Physics*

<u>*INTERNSHIP PROPOSAL*</u>

Laboratory name: Laboratory Gulliver, ESPCI
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Internship location: Laboratory Gulliver, ESPCI
Thesis possibility after internship: YES
Funding: YES

Self-replicating Materials

The next generation of materials is expected to have unprecedented functionalities, like those that already exist in biological systems. To be able to discover and produce novel advanced materials we need new paradigms for their synthesis. Fabrication of materials through the process of self-replication is one such paradigm. In general, the self-replication process starts from a template, i.e., a pre-formed object, which is introduced into a solution of building blocks, all following precise interaction rules. Free building blocks attach to specific places on the template, form bonds between themselves and eventually detach from the template, and fold into a copy of the template. The copy is ready to serve as an independent template, leading to exponential multiplication of the initial object. Over the past decade it has been demonstrated in theory and experiments how very small assemblies of building blocks can self-replicate [1-4]. However, going beyond a few building blocks has remained a formidable challenge.

We propose a new way forward, inspired by the structure of biological macro-molecules and by multivalent interactions. The main objective is to uncover design principles for self-replication of assemblies large enough to have a bulk. Using combinatorial algorithms, graph theory and state-of-the-art simulations we will systematically search for solutions that allow efficient self-replication of such assemblies. All candidate solutions will be tested in computer simulations calibrated to experiments, leading to formulation of design principles.

The internship will consist in testing a concrete replication scheme for an assembly of N=14 building blocks, one of them being in the interior of the assembly. The work will involve theoretical work coupled with numerical simulations and data analysis. We are looking for a candidate with a strong background in statistical physics and interests in programming and interdisciplinary subjects. The internship can be followed by a PhD thesis.

[1] Z. Zeravcic and M. P. Brenner, Self-Replicating Colloidal Clusters PNAS 111 (2014)
[2] H. Tanaka, Z. Zeravcic and M. P. Brenner, Mutation at Expanding Front of Self-Replicating Colloidal Clusters, PRL 117 (23) (2016)
[3] He, X. et al., Exponential growth and selection in self-replicating materials from DNA origami rafts, Nature Materials, 16 (2017)
[4] Zhuo, R. et al., Litters of self-replicating origami cross-tiles, PNAS, 116 (2019)