

INTERNSHIP PROPOSAL

(One page maximum)

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Internship location: ESPCI Paris

Thesis possibility after internship: YES

Funding: NO

If YES, which type of funding:

Folding pathways and refolding of colloidal chains

Proteins fold because the sequence of their building blocks encodes a target structure.

Colloidal chains offer a simple, controllable analogue: micrometer-sized particles linked into a flexible chain, with programmable interactions, for example through DNA coatings. When the interactions are switched on, the chain folds into a structure, and different interaction patterns favor different final geometries.

During folding the chain passes through a sequence of intermediate structures, and the number of possible intermediates grows combinatorially with chain length. The pathways the chain takes through this landscape determine whether it reaches its target or gets trapped in another structure. Controlling folding therefore means controlling pathways, not only the final energy.

In recent work, we trained a reinforcement learning agent to control the chain during folding. The agent reaches target structures with higher yield than the best temperature protocols, and it acts at specific moments of folding, much as chaperones intervene in protein folding. This raises the question of where along the pathways the outcome is decided.

In this project you will use simulations and reinforcement learning to find out which intermediate structures decide whether the chain reaches its target and how. You will then extend this to refolding, where the chain switches between structures on demand, so that shape change becomes a function. Such reconfigurable chains are a route toward micromachines: experiments can already build folding chains of DNA-coated particles, and controlling how they refold is the next step toward structures that move, grasp or switch in response to signals.

[1] R. van Mastrigt and Z. Zeravcic, <https://arxiv.org/pdf/2608.28554>

[2] A. McMullen, M. Muñoz Basagoiti, Z. Zeravcic and J. Brujic, *Nature* **610**, (2022).

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: NO

Soft Matter and Biological Physics: YES

Quantum Physics: NO

Theoretical Physics:

YES