Dr Chiara Cardelli

Theory and simulations of designable modular bionic proteins

Supervisor: Prof. Christoph Dellago

Abstract:

Self-assembly has a large number of potential applications, such as active response to the environment or catalysis, that makes it a most researched feature in material science.

Heteropolymers are important examples of self-assembling systems, where the structure is determined by the sequence along the chain of an alphabet of building blocks. Getting inspiration from natural self-assembly heteropolymers (proteins), I show computationally the design of the first artificial heteropolymers that both form precise predetermined structures and have a high variability of these structures.

I introduce a computational method to measure the minimal alphabet necessary to design the polymer. Moreover, I introduce a simple and experimentally accessible criterion to discriminate a priori designable from not-designable polymer backbones. The latter two tools can guide the engineering of new self-assembling heteropolymers that will open new applications for polymer-based materials science.

Finally, I present a computational study of designed heteropolymer conformations with complex knotted topologies.