DNA origamis: mechanisms of formation and melting, structure fluctuations.

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In this communication, we focus on the process of DNA-origami formation. In order to do this, several formation-melting experiments have been performed, where we keep track of the UV absorption as a function of the temperature. In parallel, for the melting process, we also image the resulting structures by AFM. These experiments show that, for the usual cooling-heating speed reported in most publications, folding of the origami shows hysteresis. The melting process is characterized by two transition temperatures correlated with the GC content of the staple strands and a third one at a higher temperature that may be correlated with the Origami structure. However, when the origami is prepared under constraint, the third transition disappears. During the formation of the origamis, only two transitions are observed, correlated with the GC content. In order to get further insight in the formation process, we also consider the folding-unfolding properties of a set of three ssDNA as a simplified model of origami (see figure). Using numerical simulations compared to melting experiments, we discuss entropic and defect contributions during the DNA-origami folding and the influence of a cooperative process.

In a separate study, we study the thermal fluctuations of a rectangular origami using a rigid base approximation. To do this, we use a simplified, yet accurate, model of DNA: the Stack of Plates (SOP) model [1], designed to model DNA at the base-pair level. In the SOP model, the right handed DNA structure is the result of the competition between two forces (stacking of the base pairs and a harmonic constraint to mimic sugar-phosphate backbones) and an additional simple geometric constraint. Monte-Carlo simulations show that the equilibrium conformation of the Rothemund origamis is not planar but slightly twisted. The same simulations allow to quantify the predominant elastic modes and the bending elasticity constant. We also discuss how this information can be used to design 'self-constrained' versions of the otherwise 'planar' structures.

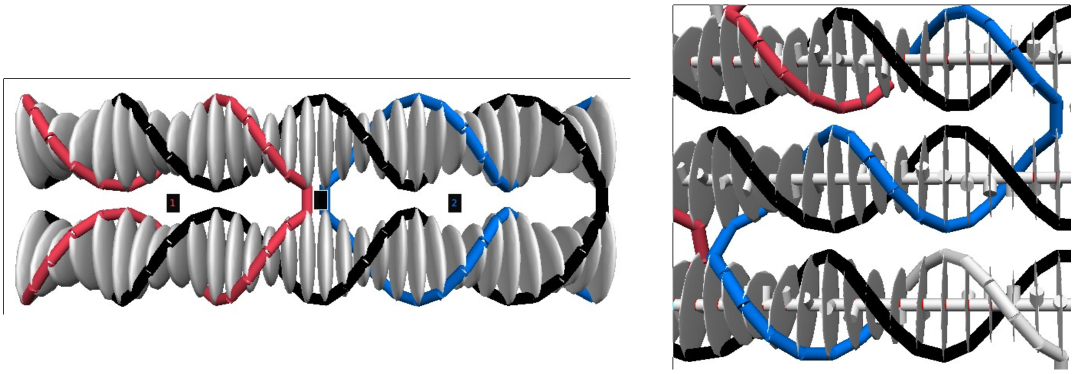

Figure : left: Simplified Origami made of 64 bases (black line) and two 32 bases long staples (red and blue lines). Right : Rectangular Origami Virus black line, staples red and blue lines.

[1] Modeling DNA structure, elasticity, and deformations at the base-pair level. Mergell, B.; Ejtehadi, M.R.; Everaers, R