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Predicting the mechanical properties of DNA-based nanostructures

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Structural DNA nanotechnology offers versatile methods to design complex three-dimensional shapes at the nanometer scale. While there has been a significant research progress in folding DNA into target shapes [1-3], little research effort has been focused on controlling the mechanical properties of these structures [4], which is essential, for example, for the design of functional materials. Here, we introduce our computational framework to predict the mechanical properties of DNA-based nanostructures that employs the finite element method. To illustrate, the bending and torsional rigidity of 6-helix DNA nanotube are predicted and compared with the experimental rigidities as well as those calculated using conventional cylinder models. We will also briefly discuss the effect of the mechanical properties of DNA structural motifs including crossovers and nicks on the mechanical properties of the entire structure.

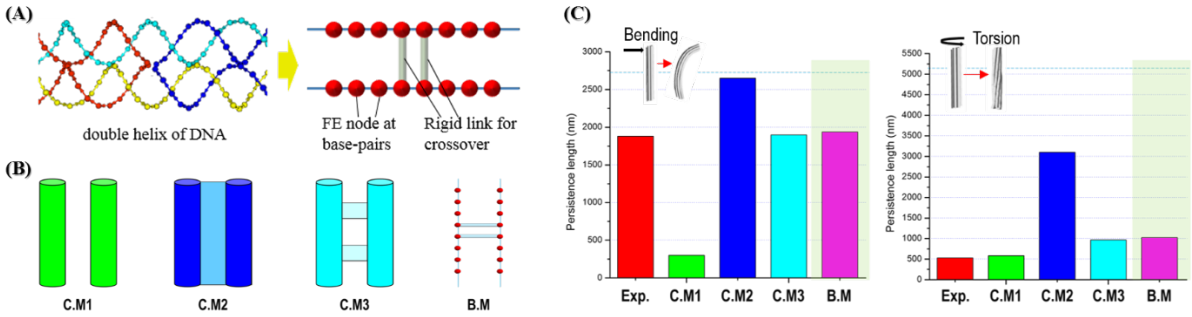

Fig. 1 (A) Finite element model for DNA origami nanostructures. (Left) Atomic structure and (Right) finite element model (B) Computational models for 6-helix DNA nanotube. C.M1~C.M3 represent the cylinder model(C.M): without the connection(C.M1), with continuous wall(C.M2) and discretized connectors(C.M3). B.M is beam model(B.M). (C) Predicted bending (left) and twist (right) rigidities. Red bars represent experimental rigidities[4]. The dashed orange lines represent the expectation from calculating the area and polar second moment of inertia..

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