Free-form DNA Origami design and higher order DNA origami communication systems

Wolfgang G. Pfeifer[1], Chao-Min Huang[2], Marcello DeLuca[2], Michael G. Poirier[1], Gaurav Arya[2] and Carlos E. Castro[1]

[1]The Ohio State University, USA, [2]Duke University, USA

Structural DNA nanotechnology has advanced rapidly in the past decade. One key for this success is the development of design approaches and software tools to guide and facilitate the complex and tedious design process. Here, we present an updated version [1] of our recently published magicDNA design-software. [2] We aim to further increase the design space, even for non-experts, and to lower the barrier for the development of highly sophisticated structures with freeform curvature. We realize the curvature of the target shape by automatically calculating the required edge gradients and orientation of each bundle along a spline. GUI based, stepwise design allows for a high level of automation, while the user maintains the ability to control and fine tune individual parameters. We automate the generation of oxDNA input files, facilitating coarse-grained simulations to evaluate the design and tune structure or properties through iteration. We have validated multiple free-form structures computationally and additionally, folded them in the laboratory. Characterization of the structures was performed by electron and atomic force microscopy, showing great agreement between design input, simulation results and structure formation (Fig. 1).

We leverage our complex design capabilities to develop multi-component dynamic devices that can exhibit collective behaviors. We demonstrate the higher order assembly of multi-component dynamic devices into linear filaments with two target functions: signal transduction and cooperative conformational changes. The signal transduction assemblies can be triggered specifically at one end by an external stimulus, and we aim to communicate a signal through a sequence of conformational changes of dynamic modules within the filament assembly. In the cooperative superstructures, each subunit conformation affects its neighbors' states using spinning components, which interact with each other. [3] These examples illustrate tremendous potential of dynamic DNA nanodevices for robotic devices and materials.

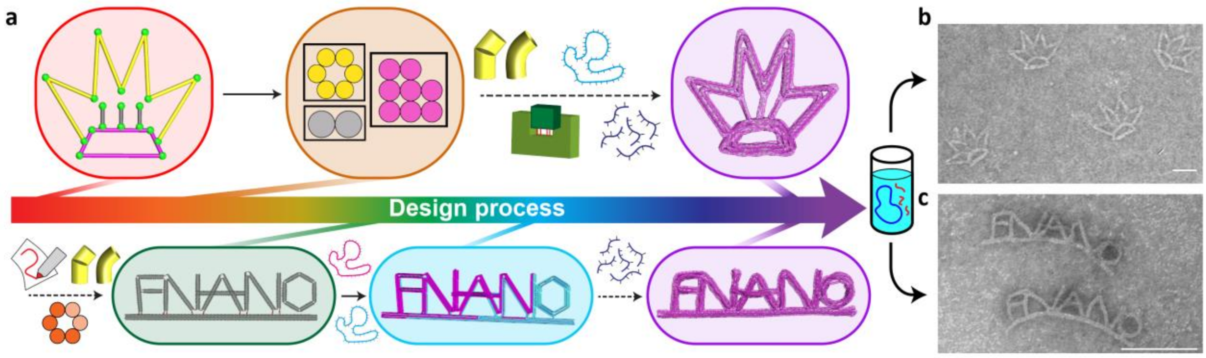

Fig. 1: Design, simulation (a), and realization of a DNA origami crown (b) and FNANO-script (c).

[1] Pfeifer, W.G., Huang, CM., Arya, G., Castro, C.E., Free-form DNA origami design with various cross-sections (in preparation)

[2] Huang, CM., Kucinic, A., Johnson, J.A. *et al.* Integrated computer-aided engineering and design for DNA assemblies. Nat. Mater. **20**, 1264–1271 (2021)

[3] DeLuca, M, Pfeifer, W.G., Castro, C.E., Arya, G., Directionally Interacting Rotor Arrays Exhibit Thermally Switchable Pattern Formation from Simple Unit Cells (in preparation)