Coarse-grained modelling for DNA nanotechnology with oxDNA

Jonathan P. K. Doye[1]

[1] *Physical & Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, South Parks Road, Oxford OX1 3QZ, United Kingdom*
Email: jonathan.doye@chem.ox.ac.uk

OxDNA is a coarse-grained model of DNA at the nucleotide level that has been parameterized to reproduce the structural, mechanical and thermodynamic properties of DNA [1]. The code that we use to simulate the model (including both molecular dynamics and Monte Carlo) is publicly available [2] and the model has also been incorporated into LAMMPS [3]. The model has been used to explore a wide range of biophysical properties of DNA and many DNA nanotechnology systems. In this talk I will review some of the recent applications of oxDNA to DNA nanotechnology. This will include characterizing the basic structural properties of DNA origami [4], and example applications to more complex origami, including those with flexible components [5] and internal stresses. The model can also be used to characterize the mechanical properties of DNA nanostructures, both in the elastic regime and their modes of failure under tension [6]. The model is also able to provide insights into the self-assembly dynamics of DNA nanostructures from the complete assembly of small DNA tetrahedra to the details of staple binding in origami [7] and even the oligomerization of DNA origami (see Figure 1). Combined with classical density functional theory, oxDNA has also been used to predict the cholesteric liquid-crystalline properties of chiral elongated DNA origami [8].

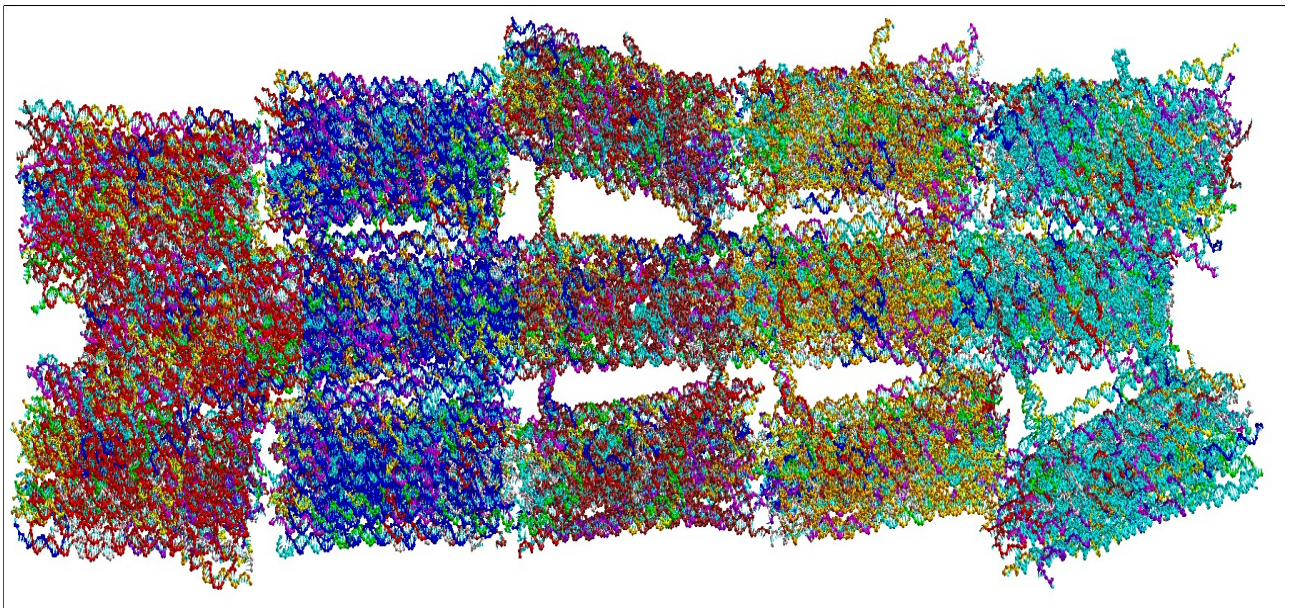

Figure 1: An oxDNA representation of a 5-mer of a DNA origami designed by the group of Lawrence Lee to undergo self-limited oligomerization due to the build-up of stress.

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