"Coarse-grained Modelling of DNA for Biophysics and Nanotechnology"

by

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Abstract:
The remarkable ability of biological matter to robustly self-assemble into well defined composite objects excites the imagination, suggesting that these processes could perhaps be emulated through the judicious design of synthetic building blocks. DNA is a particularly promising candidate for large-scale self-assembly because the specific binding of DNA bases can be accurately designed to build dynamic structures at the nanoscale.
We have developed a coarse-grained model of DNA that is simple enough to be tractable, but complex enough to capture structural, thermodynamic and mechanical properties of DNA that are crucial to DNA nanotechnology. We have used it to study basic biophysical properties of DNA such as hybridization and the stacking transition in single-stranded DNA, the response of DNA to tension leading to overstretching of double-stranded DNA and unstacking in single-stranded DNA, the response of DNA to twist, leading to bubble, cruciform and plectoneme formation, and the effect of topology on self-assembly processes. Applications to nanotechnology include DNA nanotweeze, DNA displacement reactions, a two-footed DNA walker, a burnt bridges motor, and DNA origami.

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