Energetic preference and topological constraint effects on the formation of DNA twisted toroidal bundles

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DNA toroids are compact torus-shaped bundles formed by one or multiple DNA molecules being condensed from the solution due to various condensing agents. It has been shown experimentally that the DNA toroidal bundles are twisted [1]. However, the global conformations of DNA inside these bundles are still not well understood. In this study, we investigate this issue by solving different theoretical models for the toroidal bundles and performing replica-exchange molecular dynamics (REMD) simulations for self-attractive stiff polymers of various chain lengths. We find that a moderate degree of twisting is energetically favorable for toroidal bundles, yielding optimal configurations of lower energies than in other bundles corresponding to spool-like and constant radius of curvature arrangements. The REMD simulations show that for relatively short chains, the ground states of stiff polymers are twisted toroidal bundles with the average twist degrees comparable to those obtained by the theoretical model. For a relatively long chain of 512 beads, the simulations can find only the lowest energy toroidal bundle with a low degree of twisting, indicating a problem of dynamical accessibility due to the topological constraints of the polymer. Interestingly, we also observed significantly twisted toroidal bundles with sharp U-turns in the conformation of the polymer. It is suggested that these U-turns make the formation of twisted bundles easier by effectively reducing the polymer length. This effect can be equivalent to having multiple chains in the toroid. The stability of twisted toroidal bundles may have implications for gene delivery applications.

References

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