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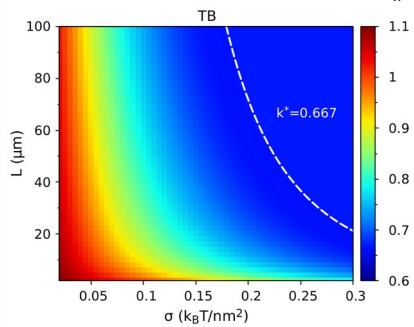
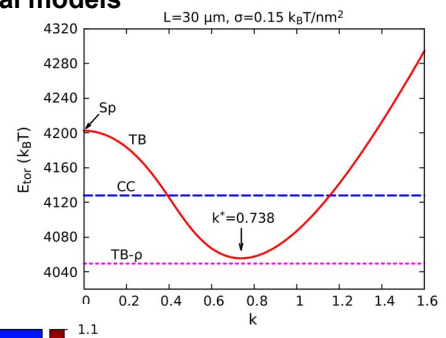
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DNA toroids are compact torus-shaped bundles formed by one or multiple DNA molecules being condensed from the solution due to various condensing agents. It has been shown that the DNA toroidal bundles are twisted. However, the global conformations of DNA inside these bundles are still not well understood. In this study, we investigate this issue by solving different 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. The simulations show that the ground states of the stiff polymers are twisted toroidal bundles with the average twist degrees close to those predicted by the theoretical model. Constant-temperature simulations show that twisted toroidal bundles can be formed through successive processes of nucleation, growth, quick tightening, and slow tightening of the toroid. The two last processes facilitate the polymer threading through the toroid's hole enabling the twisted bundle formation. The simulations also find twisted toroidal bundles with a sharp U-shaped region in the polymer conformation. It is suggested that this U-shaped region makes the formation of twisted bundles easier by effectively reducing the polymer length. This effect can be equivalent to having multiple chains in the toroid.

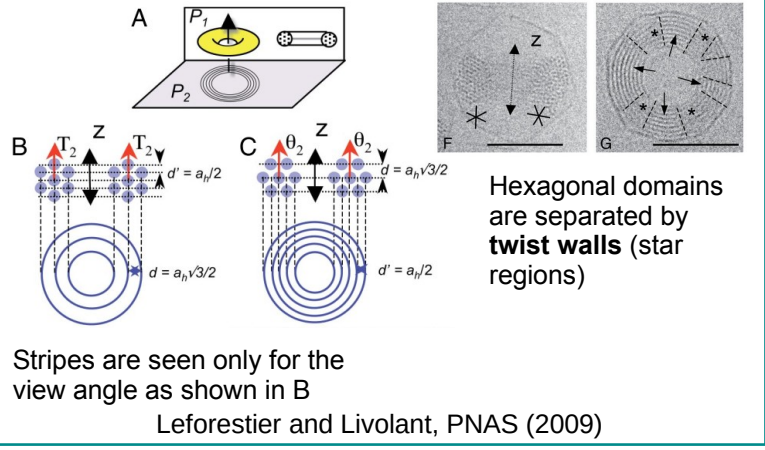
Results of the theoretical models

The twisted bundle Model (TB) yields lower energy than the spool (Sp) and constant radius of curvature (CC) models



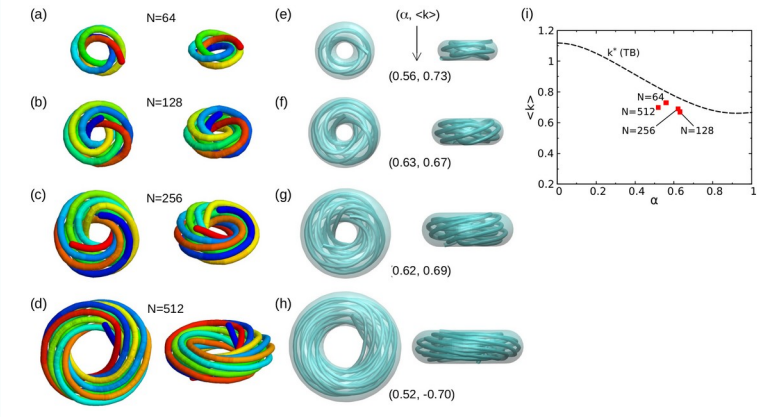
k^* values are ranged between 0.66 and 1.12

CryoEM experiments suggest that DNA toroidal bundles are twisted



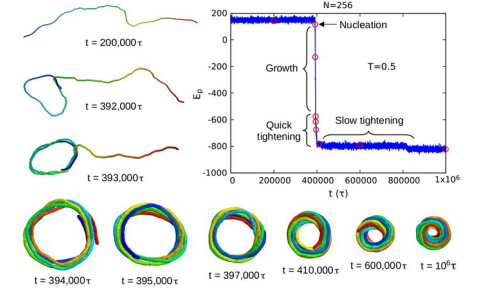
Simulations of semiflexible polymers

Lowest energy conformations obtained by REMD simulations

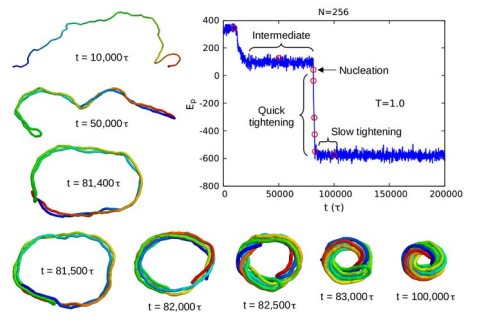


Dynamics of toroid formation: **twisted bundle formation is facilitated by the tightening processes !!**

- Direct pathway



- Indirect pathway



Twisted bundle model of DNA toroid

