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Metastable Tight Knots in DNA¹ LIANG DAI, Singapore-MIT Alliance for Research and Technology, C. BENJAMIN RENNER, PATRICK DOYLE, Department of Chemical Engineering, Massachusetts Institute of Technology — Knotted structures can spontaneously occur in polymers such as DNA and proteins, and the formation of knots affects biological functions, mechanical strength and rheological properties. In this work, we calculate the equilibrium size distribution of trefoil knots in linear DNA using off-lattice simulations. We observe metastable knots on DNA, as predicted by Grosberg and Rabin. Furthermore, we extend their theory to incorporate the finite width of chains and show an agreement between our simulations and the modified theory for real chains. Our results suggest localized knots spontaneously occur in long DNA and the contour length in the knot ranges from 600 to 1800 nm.

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