

Abstract Submitted  
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**Understanding of knots in polymers by a unified theory**<sup>1</sup> LIANG DAI, Singapore-MIT Alliance for Research and Technology, PATRICK DOYLE, MIT — Knots can occur in DNA and other polymers, in particular, for long polymers. Our research addresses two questions: what are the probabilities of random knots, and what are the typical knot sizes? In statistical physics, these two questions are related to the free energy cost of knot formation as a function of knot size. Using computer simulation as well as a unified theoretical framework based on the free energy expression of knot formation, we investigated knots under various conditions: semiflexible chains, flexible chains, polymers in confinement, and polymers with various intra-chain interactions. Several counterintuitive phenomena were obtained and explained, e.g. existence of metastable knots, knot shrinking by intra-chain repulsion. These predictions can be validated by experiments and may have impacts on DNA behaviors in vivo.

<sup>1</sup>National Research Foundation of Singapore

Liang Dai  
Singapore-MIT Alliance for Research and Technology

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