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Large-scale structural transitions in supercoiled DNA revealed by coarse-grained simulations BRAD KRAJINA, ANDREW SPAKOWITZ, Stanford Univ — Topological constraints, such as DNA supercoiling, play an integral role in genomic regulation and organization in living systems. However, physical understanding of the principles that underlie DNA structure and organization at biologically-relevant length-scales remains a formidable challenge. We develop a coarse-grained simulation approach for predicting equilibrium conformations of supercoiled DNA. With this approach, we study the conformational transitions that arise due to supercoiling across the full range of supercoiling densities that are commonly explored by living systems. Simulations of ring DNA molecules with lengths up to the scale of topological domains in the E. coli chromosome (∼10 kilobases) reveal large-scale structural transitions elicited by supercoiling, resulting in 3 supercoiling conformational regimes: chiral coils, extended plectonemes, and branched hyper-supercoils. These results capture the non-monotonic relationship of size versus degree of supercoiling observed in experimental sedimentation studies of supercoiled DNA, and our results provide a physical explanation of the structural transitions underlying this behavior.

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