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Torque-driven supercoiling transition in open DNA polymers

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In this work, we combine coarse-grained Brownian dynamics simulations and mean-field theory to study supercoiling dynamics, as well as the steady-state profiles of twist and writhe, in an open DNA polymer where one of the free ends is subjected to a constant torque. Even though the other end is free, and hence can spin and release torsional stress, we observe that the entire chain transitions between a swollen and a plectonemic phase as the torque increases beyond a critical threshold. In the plectonemic phase, we observe a non-linear twist profile in the steady state, resulting from the mutual interconversion between the injected twist and geometrical writhe, which distributes inhomogeneously along the chain. We also show that the non-equilibrium dynamics of twist accumulation is diffusive, and that writhe diffusion is negligible in this geometry, as plectonemes remain localised near the end that is being rotated. We discuss the feasibility of testing our results with single-molecule experiments.

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