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OxDNA3: A Coarse-Grained DNA Model with Sequence-Specific Curvature and Elasticity

OxDNA2 is a prominent coarse-grained DNA model that supports research in biophysics, materials science, and nanotechnology across both academic and industrial settings. While it accurately captures the thermodynamics of duplex formation and provides a reliable representation of the average geometric and mechanical characteristics of both single and duplex DNA, it currently overlooks sequence-specific structural properties. These include sequence-specific curvature and flexibility, crucial for several biological and mechanical processes. In this work we implement the next generation of the model, oxDNA3, which retains its accurate description of the thermodynamics of duplex formation, while introducing sequence-specific curvature and elasticity.

Role

Post Doc

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