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Mesoscale Modeling of Chromatin Folding[1]

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Eukaryotic chromatin is the fundamental protein/nucleic acid unit that stores the genetic material. Understanding how chromatin fibers fold and unfold in physiological conditions is important for interpreting fundamental biological processes like DNA replication and transcription regulation. Using a mesoscopic model of oligonucleosome chains and tailored sampling protocols, we elucidate the energetics of oligonucleosome folding/unfolding and the role of each histone tail, linker histones, and divalent ions in regulating chromatin structure. The resulting compact topologies reconcile features of the zigzag model with straight linker DNAs with the solenoid model with bent linker DNAs for optimal fiber organization and reveal dynamic and energetic aspects involved.

[1] In collaboration with Gaurav Arya, S. Grigoryev, S. Correll, and C. Woodcock.