

Abstract Submitted
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Modeling the dynamics of the nucleosome at various levels.¹
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ADAMS, Virginia Tech — The primary level of DNA compaction in eukaryotic
organisms is the nucleosome, yet details of its dynamics are not fully understood.
While the whole nucleosome must be highly stable, protective of its genetic material,
at the same time its tightly wrapped DNA should be highly accessible, easily revealing
its information content. A combination of atom-level classical molecular dynam-
ics and a course-grained continuum description provide insights into the functioning
of the system. In particular, the nucleosomal DNA appears to be considerably more
flexible than what can be expected based on its canonical persistence length. A
course-grained electrostatic model of the nucleosome explains how its stability can
be modulated with small environmental changes as well as post-translational modi-
fications. Implications for the nucleosome assembly process in *vivo* are discussed.

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