Modeling the dynamics of the nucleosome at various levels.\textsuperscript{1}
ALEXEY ONUFRIEV, ANDREW FENLEY, JORY ZMUDA-RUSCIO, DAVID 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 dynamics 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 coarse-grained electrostatic model of the nucleosome explains how its stability can be modulated with small environmental changes as well as post-translational modifications. Implications for the nucleosome assembly process in \textit{vivo} are discussed.

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