# Chromatin dynamics studied by molecular dynamics simulations and single-molecule FRET

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**Abstract**

The nucleosome, in which about 150 base paris of DNA are compacted by wrapping around a histone protein core, is the basic unit of eukaryotic genome packaging. Accessing genomic information requires disassembly of this structure, which depends on the environment, other factors bound to chromatin and on modification of histones.
In my presentation I will show recent results from our lab regarding the mechanism of nucleosome opening. Molecular dynamics simulations suggest roles for histone modifications in nucleosome dynamics, and concurrent single molecule spectroscopy experiments that use Förster resonance energy transferfor measuring distances between two fluorophores attached to the nucleosome (spFRET).
Using this combined experimental / simulation strategy, we have identified new intermediate states in nucleosome opening that could be used by proteins to access genomic DNA. Molecular dynamics simulations suggest a role for some internal arginine residues in nucleosome opening; mutating these residues strongly decreases nucleosome stability and promotes opening.

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