



قطب علمی
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سمینار هفتگی ماده چگال نرم

Rigid body molecular dynamics simulation of DNA in Nucleosome

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Nucleosome, the repeating unit of chromatin in Eukaryotic cells, is a complex of a DNA and histone octamers. We present a coarse grain model to study the mechanical and dynamical properties of Nucleosomal DNA. The effect of histone octamers considered as 14 groups of binding sites. our model reproduces the B-factor of phosphates with an acceptable accuracy. Also it predicts the twist defect location in NCP146 and NCP146b crystal structures. We used this model to study of twist defect diffusion through the Nucleosome. It is shown that after considering effect of DNA sequence we may obtain a diffusion constant for twist defect which is close to the experiments.

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