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سمینار هفتگی ماده چگال نرم

Evidences of Allosteric Interactions in the DNA Molecule

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All-atom simulations are the best approach to study the elastic behavior of short DNA Molecules. Recently Mazur has performed all-atom MD simulations to study the elastic properties of a double helical DNA fragment of 25 base pairs with the AT-alternating sequence [A. K. Mazur, Phys. Rev. Lett. , 2007]. Although the DNA in these simulations displays some characteristic features of the well known wormlike-chain model, it has some anomalous elastic properties that can not be explained by this model. For example, the persistence length of the DNA is not constant, and is increased with decreasing the DNA length. Another anomaly is that the Fourier spectrum of the minor groove profile has a peak with a period of about 8 bp. In this talk it will be shown that these anomalous properties are the consequence of nonlocal interactions between DNA base pairs. A nonlocal harmonic elastic rod model will be proposed, in which the roll angles of the different base pairs are coupled together. This model can successfully describe the observed anomalous elastic properties of DNA.

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