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Allostery in DNA Elasticity

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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, Biophys. J. , 2006]. The DNA in these simulations displays some anomalous elastic properties that can not be explained by the well known wormlike chain model. For example, the persistence length of the DNA is not constant, and is increased with decreasing the DNA length. In this talk it will be shown that this anomalous behavior is the consequence of the combined effect of nonlocal interactions between DNA base pairs, and the intrinsic curvature of DNA. A nonlocal harmonic elastic rod model will be proposed which can successfully describe the observed anomalous elastic behavior of DNA.

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