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Modeling spatial correlation of DNA deformations: Allosteric effects of DNA protein binding XINLIANG XU, JIANSHU CAO, Department of Chemistry, MIT, HAO GE COLLABORATION[1], X. SUNNEY XIE COLLABORATION[2] — We report a study of DNA deformations by a coarse grained mechanical model. Recent single molecule experimental studies show that when DNA molecule is deformed by its binding to a protein, the binding affinity of a second protein at distance L away from the first binding site is altered. To explain this observation, the relaxation of deformation along the DNA chain is examined. Our method predicts a general exponentially decaying behavior for differenct deformation modes. As an example, inter-helical distance deformation is studied in details, and is found to decay at a previously unknown lengthscale of 10 base pairs as a result of the balance between inter and intra DNA strand energy. This lengthscale is in good agreement with the said single molecule experimental observation. This model of local deformation relaxation helps us better understand many important issues in DNA such as the enhanced flexibility of DNA at short lengthscales and DNA repair mechanism inside cells.

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