Nanoscale physics

DNA double helix deformations at the nanoscale

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The accuracy of the genetic information transfer in living cells is largely due to the peculiarities of the structure and variability of the DNA double helix. One of the key properties of the double helix is the polymorphism of its secondary structure, allowing to change the macromolecule form and conformation under the influence of some external factors. The arising in this case deformations usually have nano sizes and provide wide tools in the processes of regulation and realization of genetic information. Besides, deformations of the DNA helix accompanied or induced by conformational transformations can pass on the nano scales without disturbing the double-stranded structure. Such deformation can contribute to the preservation of genetic texts, protecting them from possible emergency situations in the cell. Last times the study of DNA deformations acquires practical significance in material science due to the development of new directions used the unique accuracy of DNA structures in the formation a variety of nanomaterials with desired properties.

DNA deformations accompanying by the conformational transition have sufficiently large amplitudes of the structural elements deviation from their equilibrium position in a double helix, and therefore cannot be understood in terms of usually used elastic models of the mechanics of DNA macromolecule. In the same time, all-atomic modeling cannot often explain the physical mechanism of the complex processes of DNA fragments deformations with accounting the possible changes of the double helix conformation.

This work presents an approach to the study of the conformational induced deformations of a DNA macromolecule. The transformation of DNA structure is considered within the framework of a two-component model. One component of the model (external) describes the deformation of the macromolecule, as in the model of the elastic rod, another component (internal) - changes in the conformation of the monomer units of the macromolecule. Both components are regarded as coupled on the pathway of a conformational transformation [1,2].

The developed approach allows investigating the physical mechanisms of localized nanoscale deformations of the double helix due to action of small molecules, regulatory proteins, and external forces on DNA structure. The obtained results give a consistent interpretation of the observed effects of the deformability of TATA-box, A-tract, allosteric effects in DNA, and also allows explaining the threshold character of DNA unzipping and overstretching [2-5]. The approach allows to predict the size and energy of the local deformation of the double helix at the location of certain specific nucleotide sequences by their conformational states. The results obtained could be useful for the development of modern technologies in the field of molecular medicine, and DNA-based engineering as well.

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