Electronic states of DNA

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In this talk I will illustrate some of our recent results concerning the electronic states of DNA on the basis of *ab initio* quantum-chemical calculations. Recent advances in the methodologies of *ab initio* calculations for biomolecules[1] have attracted much attention to theoretical analysis of the structures, dynamics and functions of proteins. In comparison to proteins, nucleic acids such as DNA and RNA have some salient characteristics which provide unique and interesting issues for investigations. Examples include the electric conductivity or electron transfer properties of DNA strands and the importance of electron correlation effects governing the structural properties of nucleic acids, which we will focus on.

We have carried out a number of theoretical modelings for the electron transfer and electric conductivity of DNA. The electrochemical DNA chip is a very important and interesting research target because it can recognize the sequence of nucleotide base by detecting the presence of base mismatch or distingushing between single and double strands. In addtion to a phenomenological analysis,[2] we have performed microscopic calculations in which the DNA conductance was estimated on the basis of Kubo[3,4] or Landauer[5,6] formula; the structural changes of DNA chains were taken into account through the molecular dynamics simulations in aqueous solution. The electron transfer dymanics of DNA have also been investigated focusing on the solvent[7] and nuclear quantum[8] effects, which were compared well with experimental results.

We have also analyzed the electronic states of DNA on the basis of the fragment molecular orbital (FMO) method,[1] which have recently been developed for performing the *ab initio* quantum-chemical calculations for huge biomolecules. We have applied the FMO method to the complexes of DNA and estrogen receptor (ER)[9,10] and cAMP receptor protein (CRP),[11] and studied the molecular mechanism of specific sequence recognition. The significances of hydrogen bonding, charge transfer and induced polarization (dispersion) have thus been elucidated, demonstrating the necessity of accurate (correlated) quantum-chemical calculations. These effects also play important roles for sustaining the stable structures of DNA-containing systems.

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