Effects of DNA-Induced Confinement on Interaction with Metallic or Molecular Flexible Counterions

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DNA is a polyelectrolyte macromolecule with a double helical form, stabilized by water molecules and positively charged metal and molecular ions (counterions). The counterions neutralize the negative charge of DNA, forming an ion-hydration shell around the double helix. The structure of the DNA double helix causes the confinement of the ions localized in the outer and inner regions of the macromolecule. Despite the extensive number of studies on the DNA-ions system,[1] the effects of DNA-induced confinement on the structural and dynamical features of counterions around the double helix are not completely understood. In the presentation, the problem of DNA-counterion interaction will be reviewed, beginning with the earliest research papers related to the modeling of the system at the atomistic level[2] up to the most recent results[3-8]. The prominent effects due to the increased confinement induced by the DNA structure will be emphasized. Specifically, the effects of hydration of metal ions (Li^+, Na^+, K^+, Rb^+, Cs^+, Mg^{2+}) localized in different regions of the DNA macromolecule will be discussed,[4,5] as well as the conformational effects for molecular ions (putrescine^{2+}, spermidine^{3+}, and spermine^{4+}).[6,7,8] The presented results are of interest in understanding the physical mechanisms of DNA's biological functioning and the development of DNA-based materials for nanotechnological applications.

References

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