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Effects of metallic and molecular counterions in structural dynamics of the DNA double helix

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The structure of the DNA double helix is stabilized by water molecules and positively charged metallic or molecular ions, which form an ion-hydration shell around the macromolecule. The ions neutralize the negatively charged phosphate groups of the DNA backbone and thus act as counterions. Despite the extensive number of experimental and theoretical studies, the specific effects of counterions on the structural dynamics of the DNA double helix and its ion-hydration shell remain incompletely understood. This contribution will overview the most recent findings on this topic based on molecular dynamics simulation results. Specifically, the effects of hydration of Li^+, Na^+, K^+, Rb^+, Cs^+ and Mg^{2+} counterions localized in different regions of the DNA macromolecule will be discussed, along with the interplay of water molecules around the ions and within the hydration shell of the double helix [1,2]. In the case of molecular ions, the role of conformational effects of flexible polyamines (putrescine^{2+}, spermidine^{3+}, and spermine^{4+}) for the interaction with the DNA double helix and the formation of stable DNA-DNA contacts will be described [3-6]. The results will be discussed in the context of understanding the physical mechanisms behind DNA's biological functioning and the development of DNA-based materials for nanotechnological applications.

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