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Counterions in DNA-Nanomaterials

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The DNA molecule consists of chains of nucleotides that, under physiological conditions, are bound by hydrogen bonds and form a double helix. The nitrogenous bases are located inside the helix, whereas the phosphate groups are exposed to the surrounding aqueous environment. This structural organization arises from the hydrophobic nature of the bases and the hydrophilic character of the phosphate groups. DNA phosphates carry a negative charge and are neutralized in solution by positively charged ions, known as counterions, which may be metal ions or molecular ions. Beyond its fundamental biological role, DNA possesses unique physical properties that make it attractive as a material for nanotechnological applications. Consequently, the fundamental properties of DNA-counterion systems are of considerable interest.

In this presentation, the results obtained using theoretical models, classical molecular dynamics simulations, and quantum chemical calculations for DNA in the presence of counterions will be discussed. In particular, DNA condensation induced by counterions of different valencies will be examined. DNA is known to condense in the presence of multivalent ions such as spermidine3+ and spermine4+, primarily due to effective charge neutralization, whereas condensation is usually not observed with monovalent ions like sodium or potassium. The analysis emphasizes that differences in DNA-counterion interactions are strongly influenced by the structure of the ion hydration shells and the ability of ions to form stable complexes with atoms of the DNA macromolecule. Understanding these hydration effects is essential for controlling the physical properties of DNA-ion systems and for the design of DNA-based nanomaterials.

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