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In search of Physics of Interactions for Silver ion with single-strand DNA scaffold: A combined Molecular Dynamics Simulations and Experimental Analysis

Understanding the physical and molecular mechanism of the interaction of surfaces, nano- and microparticles with DNA represents a great interest in today's biomedical applications. Nucleic acids have crucial biological functions in gene storage, replication, repair, and gene regulation. Due to the negatively charged phosphate backbones of ss-DNA, it is intrinsically polyanionic in nature. This intra-strand repulsion between specific phosphate residues in single-stranded DNA makes the whole structure stable against folding. However, charged cations (like Ag+, Hg2+, Ca2+, Na+, Mg2+, etc....) block this electrostatic attraction and aid in the structural breakdown of single-stranded DNA.

The structure and dynamics of negatively charged nucleic acids strongly correlate with the concentration and charge of the oppositely charged counterions. It is well known that the structural collapse of DNA is favored in the presence of additional salt, a source of excess oppositely charged ions. Under such conditions stranded DNA adopts a collapsed coil-like conformation, typically characterized by stacking base pairs. The dynamics further take an interesting turn when the system is introduced on a highly reactive oxide nano-surface like MoS2. The nanostructured surface affects the overall charge dynamics at the surface and the single-stranded DNA conformation. Using atomistic molecular dynamics simulation as well as experiment, we would like to explore the effect of varying salt concentration (Ag+) on the (small base sequence) single-stranded DNA conformation. In a nutshell, our experiment and simulation will explore how in the presence of silver ions, non-sequential base stacking and overcharging compete and affect single-stranded DNA dynamics.

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