these were most likely caused by the denaturation of DNA and the dissociation of the aggregate.

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Molecular Dynamics Investigations on Base Sequence Specificity of Counterion Binding to DNA
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DNA is a highly charged polymer, whose structure, flexibility and biological functionality are strongly influenced by the interactions with solvent and counterions. In recent years it has been shown that the monovalent cations, as the physiological counterions Na⁺ and K⁺ can bind directly to DNA, partially losing their hydration water. These studies have revised the common view of monovalent cations binding to the DNA double helix in a deolated manner, without dehydration and irrespective of the base sequence. However, obtaining detailed information at the atomistic level on the binding of highly mobile ions like Na⁺ or K⁺ is tricky [1,2], and often the experimental data leaves space to several interpretations. Detailed information on counterion/DNA interaction can be obtained by Molecular Dynamics simulations. Its validity has always to be carefully checked. We present here a Molecular Dynamics investigation of interactions between DNA and its counterions discussing the sequence specific interactions with alkaline ions. Studied DNA sequences. Red: Adenine; Blue: Thymine; Green: Guanine; Yellow: Cytosine.

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Improved Parametrization of Ion-DNA Interactions for MD Simulations of Dense DNA Systems
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Nucleic acids - highly charged polymers - are often densely packed in biological systems. Counterions play an essential role in the biological processes involving densely packed DNA, such as chromosome remodeling and RNA folding. However, experimental measurements of the ion atmosphere around the nucleic acids remain elusive. All-atom molecular dynamics (MD) simulations can be used to characterize the ion atmosphere in great details; however, the usefulness of such simulations depends on the accuracy of the underlying computational model. Here, we test the accuracy of the current all-atom force field by carrying out an MD simulation of 64 parallel DNA duplexes (DNA array). Undesirably, we find both DNA array pressure and DNA distributions derived from these simulations to be inconsistent with the X-ray diffraction and osmotic pressure measurements. We find that the origin of such discrepancy is inaccurate description of ion interaction with the DNA phosphate. To improve the model, we fine-tune the ion-phosphate interaction parameters to reproduce experimental osmotic pressure of binary electrolyte solutions such as Na-dimethylphosphate. Using our improved model, we characterize ionic atmosphere in the DNA array. We find Mg to exhibit much stronger affinity to the DNA than Na: the concentration of Mg and Na ions inside the DNA array are ~500 and ~700 mM, respectively, although the ion concentration outside the DNA arrays is [Mg] = 20 and [Na] = 200 mM. Residence time analysis of Na/Mg in contact with DNA phosphate supports our assertion that Mg-phosphate interaction is much stronger than Na-phosphate one. We expect our successful re-parametrization of ion-phosphate interactions to find applications in MD simulations of other nucleic acid systems, in which ion-DNA interactions are critical, such as folding of RNA, ribozyme dynamics and the molecular mechanism of translation.

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A General Model for Solute Effects: How to Predict the Effect of Any Solute on Any Process
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Small solutes affect protein and nucleic acid processes because of favorable or unfavorable chemical interactions of the solute with the biopolymer surface exposed or buried in the process. Large solutes also exclude volume and affect processes where biopolymer molecularity and/or shape changes. Here, we develop an analysis to separate and interpret or predict excluded volume and chemical effects of a flexible coil polymer on a process. We report a study of the concentration-dependent effects of the full series from monomeric to polymeric PEG on intramolecular hairpin and intermolecular duplex formation by 12-nucleotide DNA strands. We find that chemical effects of PEG on these processes increase in proportion to the product of the amount of DNA surface exposed on melting and the amount of PEG surface that is accessible to this DNA, and these effects are completely described by two interaction terms that quantify the interactions between this DNA surface and PEG end and interior groups. We find that excluded volume effects, once separated from these chemical effects, are quantitatively described by the analytical theory of Hermans, which predicts the excluded volume between a flexible polymer and a rigid molecule. From this analysis, we show that at constant concentration of PEG monomer, increasing PEG size increases the excluded volume effect but decreases the chemical interaction effect, because in a large PEG coil a smaller fraction of the monomers are accessible to the DNA. Volume exclusion by PEG has a much larger effect on intermolecular duplex formation than on intramolecular hairpin formation.