Condensed matter physics / 113

DNA condensation induced by Li^+ counterions

Authors: Tetiana Bubon; Dmytro Piatnytskyi; Sergiy Perepelytsya

Bogolyubov Institute for Theoretical Physics,National Academy of Sciences of Ukraine

Corresponding Author: dvpyat@gmail.com

DNA is a highly charged molecule that is neutralized by positively charged metal or molecular ions (counterions). The neutralization of DNA by these counterions induces various effects, including the formation of DNA-DNA contacts that lead to further condensation of the macromolecule. The effect of DNA condensation has been widely observed for highly charged counterions (≥3+). For divalent counterions, DNA condensation is sometimes observed, whereas with monovalent ions, it is generally considered impossible due to insufficient neutralization of the double helix's charge required to form stable DNA-DNA contacts. However, the idea that DNA cannot condense with monovalent ions overlooks the interplay between water molecules in the DNA hydration shell and those in the hydration shell of counterions, which can play an essential role in the interaction of DNA duplexes. Li^+ is highly hydrated and it is localized within a stable tetrahedron formed by four oxygen atoms of water molecules. Considering the structural complementarity of the DNA phosphate groups to the hydration shell of Li^+ ions [1], the formation of Li-mediated DNA-DNA contacts may occur. To elucidate the possibility of forming stable Li^+ crosslinks between different DNA double helices, the molecular mechanisms of their formation are studied in the present work. Atomistic molecular dynamics simulations of five DNA fragments in a simulation box with LiCl concentration 0.1 M and 1.0 M of salt were carried out. As a result of our study, the possible configurations of crosslinks between phosphate groups of different DNA fragments were determined. To validate the obtained results, the vibrational spectra of characteristic complexes were calculated using quantum-chemical methods and compared with existing experimental data. This work demonstrates that DNA-DNA contacts mediated by Li^+ can form in aqueous solutions with a high concentration of DNA and LiCl salt, supporting the idea of DNA condensation by Li^+ counterions.

[1] Lyubartsev, A. P.; Laaksonen, A. Molecular Dynamics Simulations of DNA in Solution with Different Counter-Ions. J. Biomol. Struct. Dyn. 1998, 16 (3), 579–592. https://doi.org/10.1080/07391102.1998.10508271.