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Dynamics of K^+ counterions around DNA double helix in the external electric field: a molecular dynamics study

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The structure of DNA double helix is stabilized by metal counterions condensed to a diffuse layer around the macromolecule. The dynamics of counterions in real conditions is governed by the electric fields from DNA and other biological macromolecules. In the present work, the molecular dynamics study was performed for the system of DNA double helix with neutralizing K^+ counterions and for the system of KCl salt solution in an external electric field of different strength (up to 32 mV/ Å). The analysis of ionic conductivities of these systems has shown that the counterions around the DNA double helix are slowed down compared with the KCl salt solution. The calculated values of ion mobility are within (0.05–0.4) mS/cm depending on the orientation of the external electric field relative to the double helix. Under the electric field parallel to the macromolecule, K^+ counterions move along the grooves of the double helix staying longer in the places with narrower minor groove. Under the electric field perpendicular to the macromolecule, the dynamics of counterions is less affected by DNA atoms, and starting with the electric field values about 30 mV/ Å the double helix undergoes a phase transition from a double-stranded to a single-strand state.

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