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Computational Investigation of Water Glass Behavior Around DNA

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INTRODUCTION

Water displays interesting and unusual physico-chemical properties, many of which are necessary for the existence of life. Among these properties is water's polyamorphism, i.e. the fact that water displays two distinct amorphous solid phases, LDA (Low-Density) and HDA (High-Density Amorphous Water). Recent experimental studies[1] have shown that, upon cooling, DNA's hydration layer is made of LDA and HDA. Motivated by such findings, we've studied the molecular dynamics of this phenomena, which could be interesting for anti-freezing technologies and cryopreservation of biological matter.[2]

METHODS

Molecular Dynamics (MD) simulations were carried out using the GROMACS 4.5[3] to study a system composed of a Dickerson-Dodecamer double strand in pure water molecules of TIP3P (called TIP3P-DNA) and TIP5P model (TIP5P-DNA) or in NaCl solution of physiological concentration (TIP5P-FISIO). The NpT ensemble was used to equilibrate the system at 300 K and then relevant dynamical and structural data was obtained by further simulation in the NVE ensemble. The system was then cooled by 10 K and the procedure repeated.

RESULTS AND DISCUSSION

Our findings show that TIP3P water is unable to produce dynamic glass transition either in bulk solution or around DNA's major and minor grooves, as shown if Figure 1. TIP5P model, however, could show such transition. It can be seen that (i) water further than 1 nm from DNA has its dynamics unaffected by the biomolecule; (ii) NaCl of physiological concentration has no relevant impact on the systems dynamics; (iii) water in DNA's grooves behaves very differently from bulk water, but similar to one another (major *versus* minor groove); (iv) groove water has non-Arrhenius dynamics; (v) in low temperatures groove water has a slower dynamic than bulk water, but, as temperature decreases, an inversion occurs.

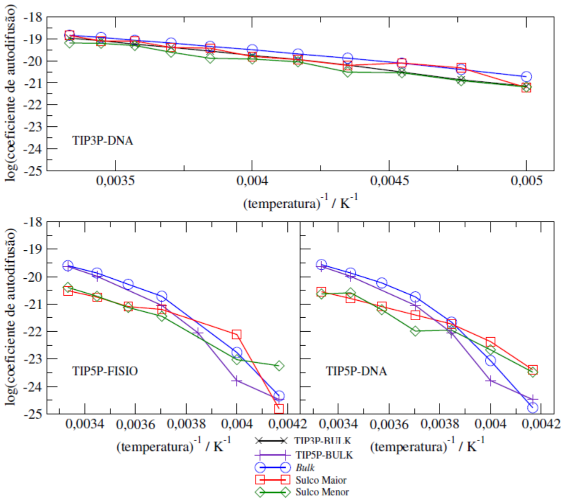

Figure 1. Arrhenius plot of logarithm of self-diffusion coefficient versus inverse temperature.

CONCLUSIONS

The simulations shows that, at low temperatures, water in DNA's grooves is more mobile than bulk water at the same temperature. This suggests a possible interpretation for the glass formation of water around DNA, as verified by experiments: water cannot properly crystalize around DNA due to the fast dynamics of water in the grooves.

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