

# **DNA AND ITS COUNTERIONS: A MOLECULAR DYNAMICS STUDY**

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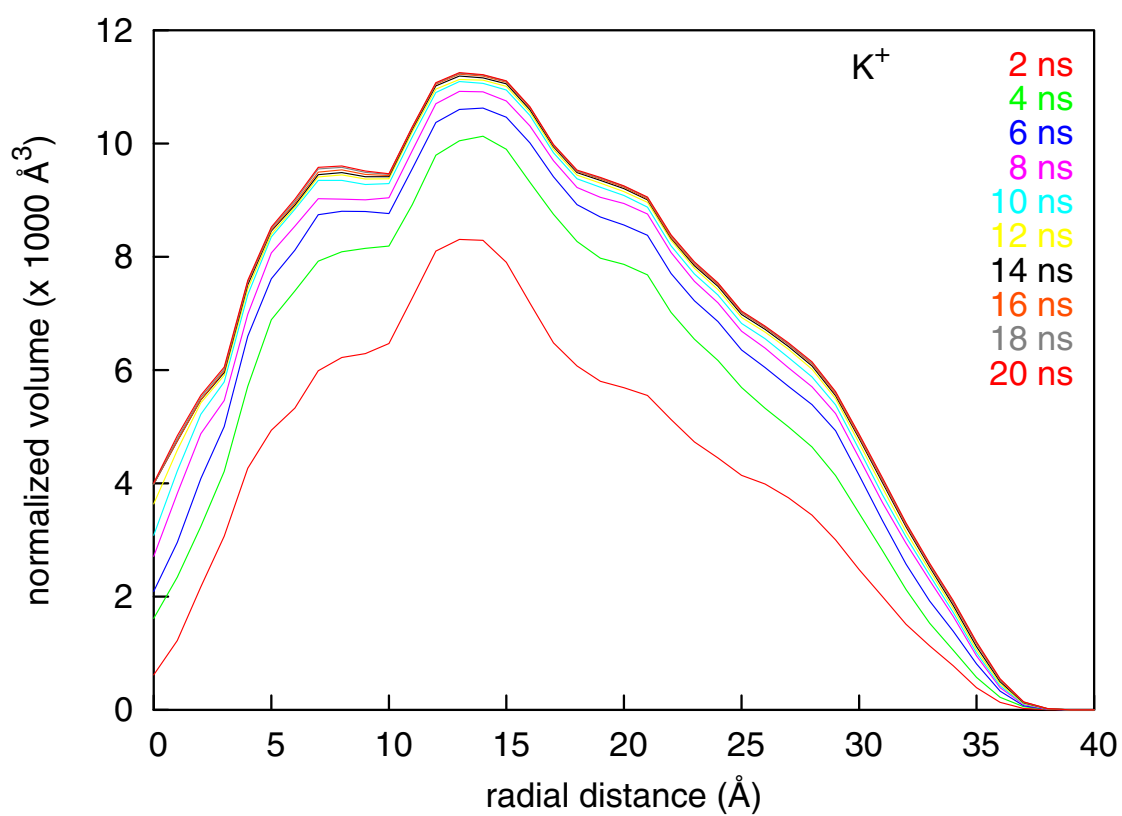
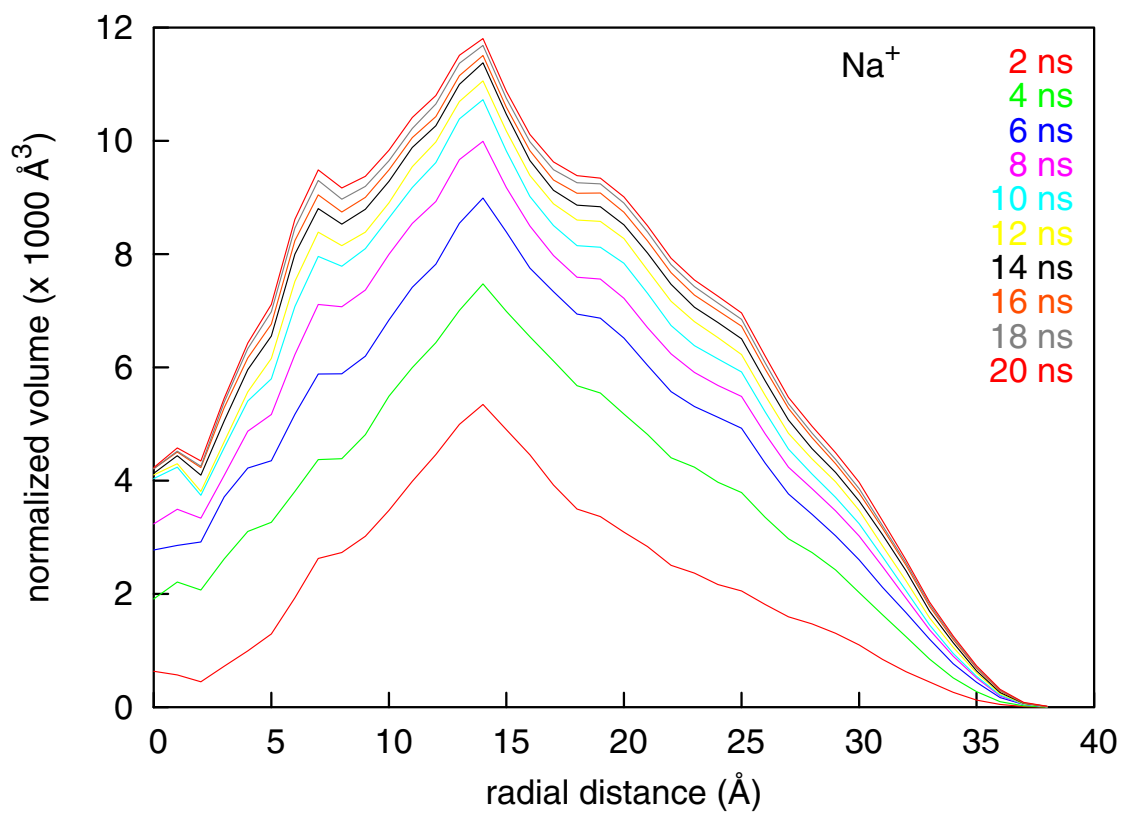
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## **Supplementary material:**

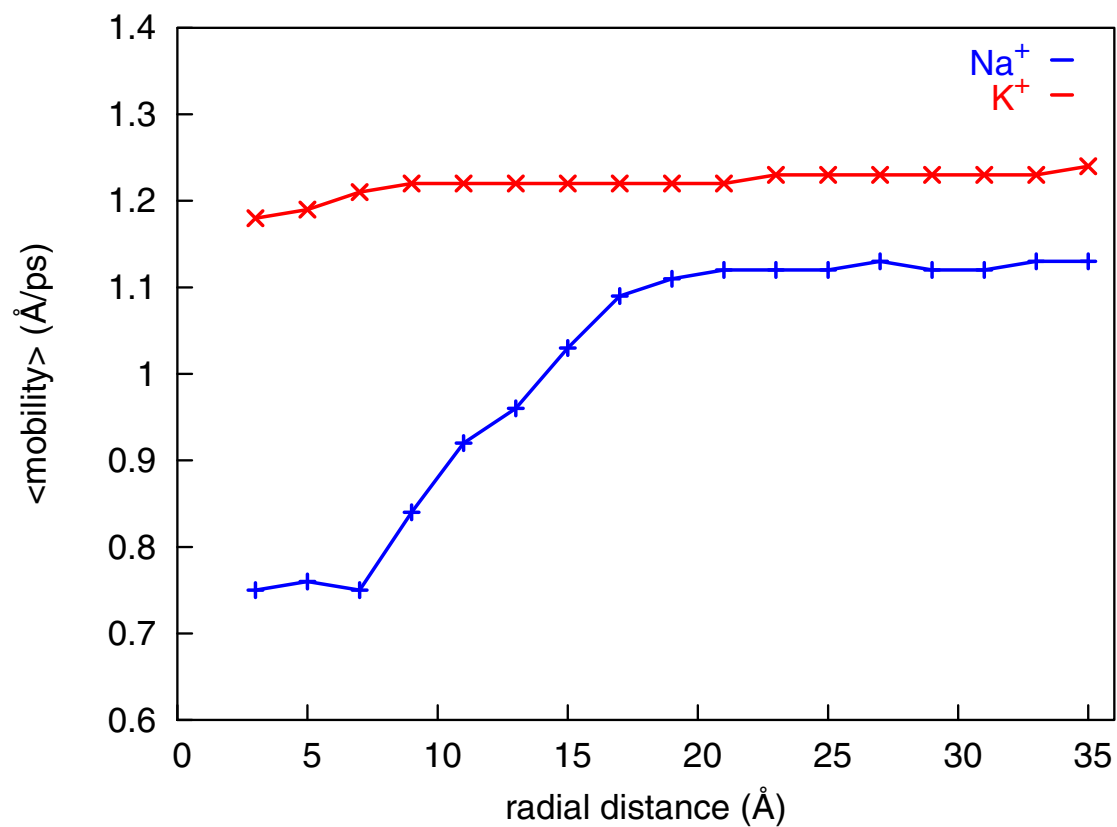
Figure S1

Figure S2

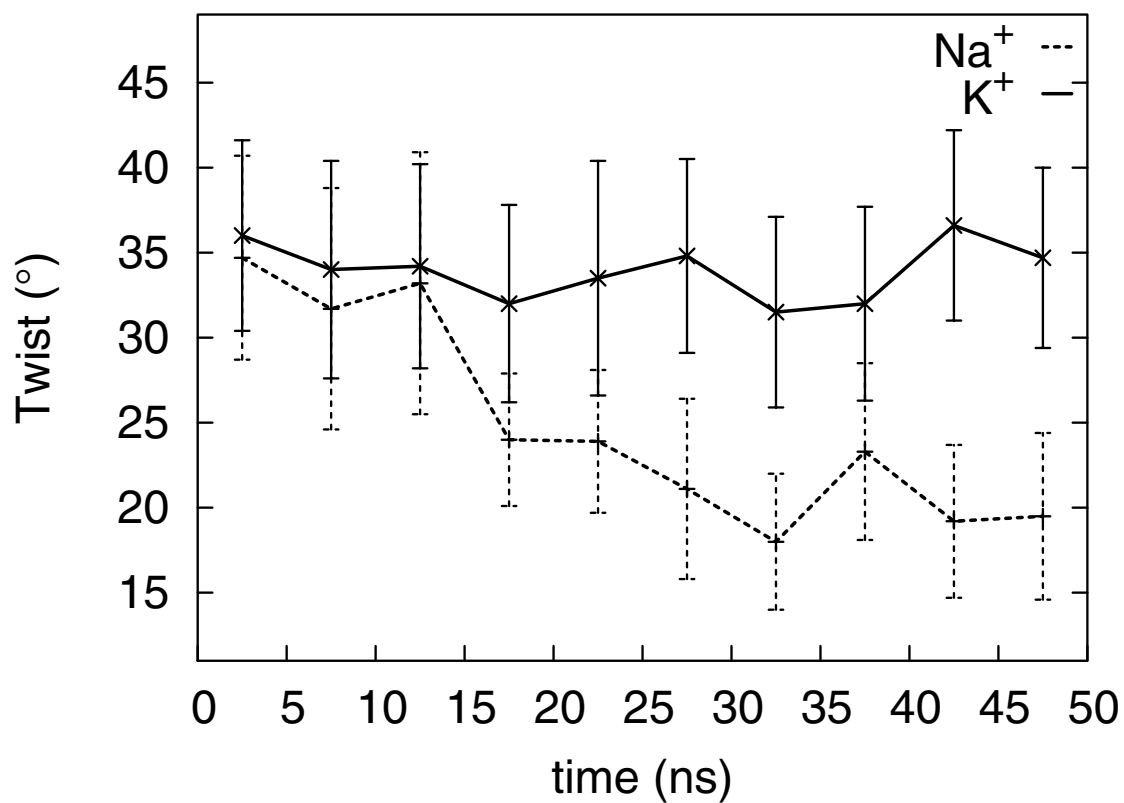
Figure S3



**Figure S1.** Normalized volume of cylindrical shells around DNA sampled by Na<sup>+</sup> (top) and K<sup>+</sup> (bottom) versus radial distance from a linear DNA axis during the first 20 ns simulation time.



**Figure S2.** Ion mobility calculated as a function of the mean distance of ions from the DNA axis over 50 ns simulation time with Na<sup>+</sup> (blue) and K<sup>+</sup> (red) counterions.



**Figure S3.** Twist angle between levels C<sub>8</sub>/T<sub>9</sub> as a function of simulation time. Average values over 5 ns with standard deviation are given for simulation with Na<sup>+</sup> (dotted line) and K<sup>+</sup> counterions (solid line).