Frequency–Dependent Permittivity of DNA using Molecular Dynamics Simulation

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We have performed a series of molecular dynamics simulation of an 8–mer DNA with water molecules, to investigate dynamic properties of DNA. The dynamic properties can be calculated according to the linear response theory, where the frequency dependent dielectric function $\varepsilon(\omega)$ is given by,

$$\varepsilon(\omega)=1+4\pi/3Vk_BT\ [\ \langle \mathbf{M}(0)\mathbf{M}(0)\rangle + i\omega\langle \mathbf{M}(0)\mathbf{M}(t)\rangle_\omega+\langle \mathbf{M}(0)\mathbf{J}(t)\rangle_\omega],$$

which is explored for several cases of aqueous–ion solutions[1][2][3]. Note that $\mathbf{M}(t)$ and $\mathbf{J}(t)$ are the total dipole moment and the total electric current of ions at time t, respectively, and $\langle\rangle_\omega$ denotes the Laplace transform. Figure 1 shows the correlation function $\langle \mathbf{M}(0)\mathbf{M}(t)\rangle$ obtained from the simulation and that of the first–order approximation

$$\langle \mathbf{M}(0)\mathbf{M}(t)\rangle=919.4\ \exp(-t/5500) + 3.6\ \exp(-t/0.8).$$

Figure 2 shows the frequency–dependent dielectric function, calculated from correlation function obtained from simulation and its first–order approximation. This shows the static dielectric constant, whose absolute value seems twice as large as the real value, according to the reference results obtained from water simulation. The simulation is still underway, so the decay of the dielectric function in the higher–frequency region is un–certain, however, the first–order approximation result shows some perspective view to them.

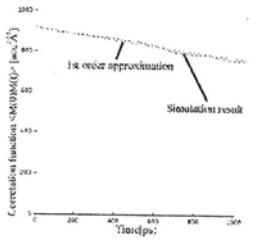

Fig1. Correlation function.

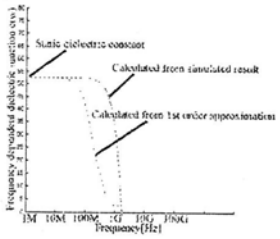

Fig.2 Dielectric function.

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[2] Gerald Loffler, etc, J. Chem. Phys., 107(8), pp. 3135–3143, 22 Aug., 1997.
[3] S. Chowdhuri, etc, J. Chem. Phys., 115(8), pp. 3732–3741, 8 Nov., 2001.