Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Humidity dependence of optical property of a DNA fiber: first-principles and molecular dynamics studies[1] TAKENORI YAMAMOTO, Faculty of Science, Toho University; IIS, The University of Tokyo, TSUYOSHI UDA, AdvanceSoft Corporation; IIS, The University of Tokyo, TAKAHISA OHNO, National Institute for Materials Science (NIMS); IIS, The University of Tokyo — We present first-principles and molecular dynamics studies for humidity dependence of optical property of a deoxyribonucleic acid (DNA) double helix fiber. The first-principles electronic structure and the molecular dynamics simulations reveal that the electronic structure of the DNA fiber is varied by the hydration amount or the relative humidity. We show that the ultraviolet optical conductivity is influenced by the hydration structure and the DNA deformation, and that our findings agree with other theoretical results and experimental observations. The infrared (IR) optical conductivity is calculated by the molecular dynamics approach. The humidity dependence of the optical conductivity due to the dipole relaxation of water is in close agreement with experimental observations. The IR absorption spectrum due to DNA vibrations agrees with the experimental spectrum in feature.

[1]A part of this research was done in RISS project supported by RDNIT of MEXT.

Takenori Yamamoto
Faculty of Science, Toho University

Date submitted: 30 Dec 2009 Electronic form version 1.4