

Abstract Submitted
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Hydration effect on optical property of a DNA fiber: A first-principles study¹ TAKENORI YAMAMOTO, Faculty of Science, Toho University and IIS, The University of Tokyo, TSUYOSHI UDA, AdvanceSoft Corporation, TAKAHISA OHNO, National Institute for Materials Science (NIMS) and IIS, The University of Tokyo — We present a first-principles study for solvation effects on properties 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 and the deformation. The electrostatic interaction in the DNA fiber is screened by the hydration water. The screened electrostatic interaction determines the electronic structure of the DNA fiber, while the electronic structure of the water is determined by its polarized change as the result of the electrostatic response. We show that the optical conductivity is influenced by the hydration and the deformation, and that our findings agree with other theoretical results and experimental observations. In conclusion, we really stress that the solvation must be carefully taken account for simulating electronic structures and properties of DNA's.

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