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QM/MM/3D-RISM study of solvation and electronic structure of DNA NORIO YOSHIDA, FUMIO HIRATA, Institute for Molecular Science — It is well known that a DNA has high electronic conductivity in wet condition, while it doesn't in dry condition. Therefore, the solvent effects on the electronic properties of DNA got much attention in the field of biology, chemistry and physics. In the present study, we employ three-dimensional reference interaction site model method combined with quantum mechanics and molecular mechanics (QM/MM) method to treat the large DNA chain in solvent. By this theory, the electronic structure of DNA and solvent distribution around DNA can be determined simultaneously. The result shows the dramatic change of electronic structure of solute DNA molecule by solvation. The change strongly depends on the sequence of DNA.

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