

Theoretical study of DNA with unnatural base pair system using order-N DFT calculations

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We present our recent theoretical study on DNA with unnatural base pair, called Ds-Pa, (7-(2-thienyl)-imidazo[4,5-b]pyridine (Ds) and pyrrole-2-carbaldehyde (Pa)) systems using our order-N density functional theory (DFT) calculations. Previously we have reported the intermolecular interactions of the unnatural base pair Ds-Pa molecule in the gas phase by DFT and HF-MP2 using the quantum chemical method [1]. We have found that the interaction between Ds and Pa molecules is very weak and mainly governed by the dispersion forces. This result suggests that the stabilization of unnatural base pair within DNA double helix structure, which is observed in experiments, should depend on the environment such as the frame spacing of DNA backbone, the interaction of the unnatural base with its upper and lower base pairs, and/or the existence of solvent.

Based on these results, we have applied our order-N DFT code, CONQUEST [2] to hydrated DNA system including one unnatural Ds-Pa base pair (see figure). The system consists of 11,912 atoms (763 atoms for a DNA including one Ds-Pa pair, 22 Na counter ions and 3,709 water molecules). We can employ accurate and robust SCF calculations on such a complex system using our order-N DFT methodology. As in our previous study on hydrated DNA systems [3], we have calculated the atomic forces and the total energies. We also discuss the van der Waals effect on the total energies and the atomic forces.

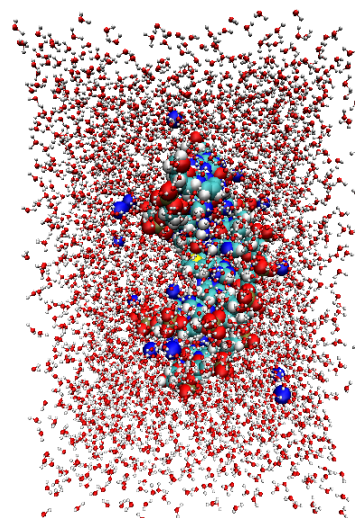


Figure.
DNA including one unnatural base pair, Ds-Pa system, which contains 11,912 atoms.

[1] T. Otsuka and T. Miyazaki, *Int. J. Quantum Chem.*, 113, 504-509, 2013.

[2] D. R. Bowler and T. Miyazaki, *Rep. Prog. Phys.* 75, 036503, 2012. See our web page; <http://www.order-n.org/>

[3] T. Otsuka, T. Miyazaki, T. Ohno, D. R. Bowler, M. J. Gillan, *J. Phys. Condens. Matter*, 20, 294201 (2008).