Intermolecular binding of DNA by FMO combined with QMC

Kousei Tsushima (0710050)

School of Information Science,
Japan Advanced Institute of Science and Technology

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This research treats a computer simulation on materials science, electronic structure calculation. Research in this field shows that there are systems which are difficult for conventional methods to deal with. These systems include intermolecular binding of biological system. The difficulty comes from the fact that intermolecular binding results from fluctuation of electronic interaction. For this reason, it is necessary to treat the electronic correlation very carefully for such systems. From this point of view, our research attempts to adopt a method which has high reliability for treating electronic interaction in *ab-initio* calculations, and apply the method to intermolecular binding.

DNA is regarded as a difficult example of intermolecular binding. In order to describe intermolecular force of DNA, the Quantum Monte Carlo(QMC) procedure is applied, and this enables us to evaluate electronic correlation with high reliability. But the calculation of a large system is a difficult problem. Since the molecular structure of biological systems is often seen as a system can often be divided into collective atoms, the whole system can be broken down into a number of smaller subsystems. The method based on this concept is Fragment Molecular Orbital method(FMO method). Thus, we attempt to apply QMC combined with FMO to the structure of DNA. As a QMC, we used Variational Monte Carlo method(VMC method).

There are two ways to analyze intermolecular binding, One is the binding curve analysis of the whole energy and the other is analysis based on InterFragment Interaction Energy(IFIE). Furthermore it was found that the binding can also be evaluated only by a energy which is a component IFIE.

Our result could not successfully express the binding, this is because the energy is evaluated each point of bias which is random effect. Altogether, specific dependency between two points was expected to be lost due to bias on the mean value. In order to improve the result, we prepared charge density, which is different from FMO-VMC's one. Specifically, we adopted charge density that was prepared by HF-SCF method, which does not use random numbers. However the results did not improve. This means that charge density was not cause of the bias.

Other ingredient causing the bias could be several corrections for the trial wave function on QMC. There are two corrections used in our calculation, the one is cusp correction and second is the optimization of Jastraw functions. To be more specific, since the optimization for such corrections are made to each point of individual form, the quality of the optimization might be not uniform. As a future work, it would be necessary, to improve these correction schemes.