2E19

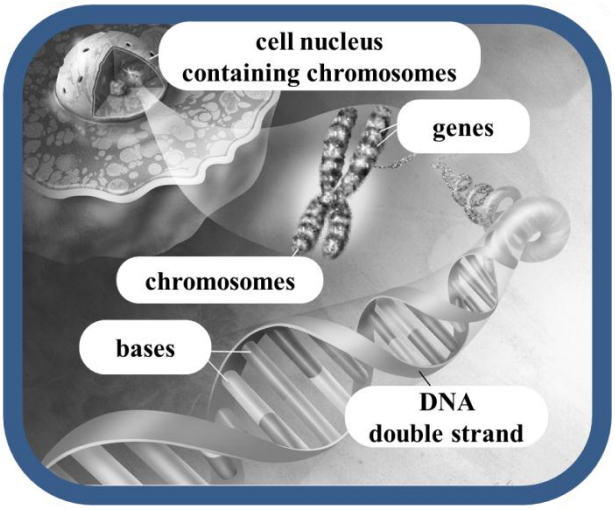
DNA の塩基対間相互作用エネルギーの高精度計算と塩基配列依存性

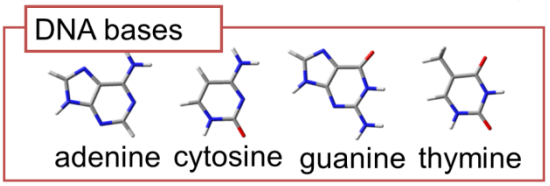
（広島大院・理，広島大 QuLiS）相田 美砂子

Ab initio MO study on the interaction energy of base-pairs in DNA

(Center for Quantum Life Sciences, Graduate School of Science, Hiroshima University)
Misako AIDA

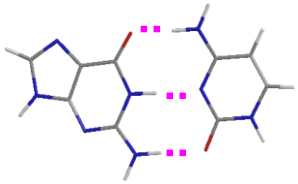
DNA is a blueprint of life. It includes all the information of life. Genetic code makes use of the base sequence. High order structure of DNA is important in transcription, expression and replication, and so on. Each person has his/her own DNA sequence: therefore, there are huge kinds of base sequence. And furthermore, DNA is too large to be a target molecule of accurate theoretical calculations. So, what can we do…?



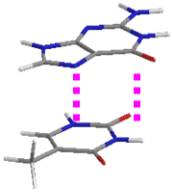


In double helical DNA, the component bases are hydrogen-bonded and are stacked, leading to the formation of enormously long DNA molecule.

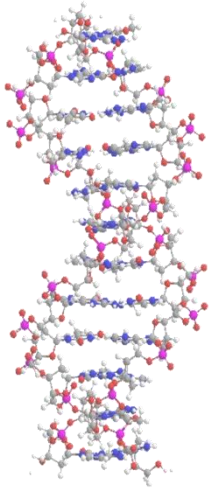
There had been many quantum chemical calculations for hydrogen bonding pairs and stacking pairs, including 2 bases.



hydrogen-bonding base-pair



stacking interaction of bases

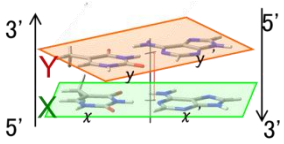


However, there had been no systematic calculations for 2 stacking base-pairs or more, including more than 4 bases. In this work, we deal with 2 and 3 stacked base-pairs. We will clarify the additivity of stacking interaction, and the importance of many-body effect.

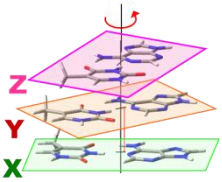
Thus, we aim at giving the smallest unit as a building block of DNA.

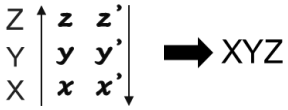
Since a Watson-Crick base pair is complementary, only one base is enough to specify the base pair. In this work, we use a small letter (***a***, ***c***, ***g***, or ***t***) to indicate a *base*, and a capital letter (**A**, **C**, **G**, or **T**) to indicate a *base-pair* (***a*-*t***, ***c*- *g***, ***g*-*c***, or ***t*-*a***).

A stacked 2 base-pairs is specified as below. We calculated the energies for all possible 10 kinds of stacked 2 base-pairs at the theoretical level of MP2/6-31G*, and 2-, 3- and 4-body interaction energies were evaluated with BSSE corrected. We calculated the energies also at RI-MP2/aug-cc-pVDZ.

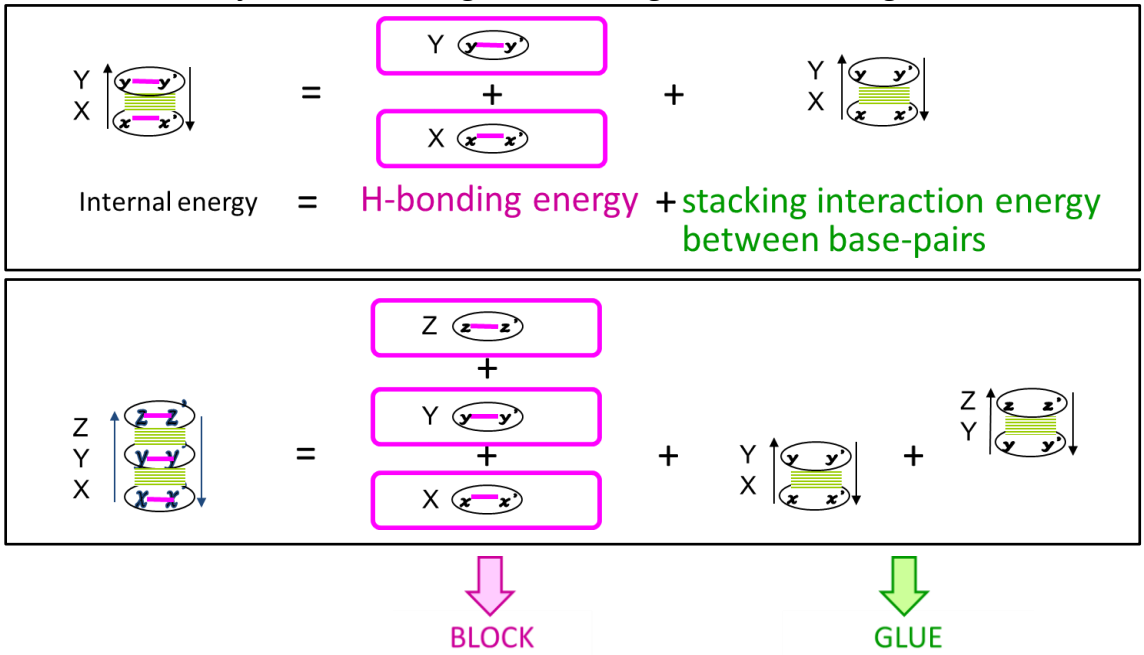


A stacked 3 base-pairs is specified as below. We calculated the energies for all possible 64 kinds of stacked 3 base-pairs at MP2/6-31G*, and 2-, 3-, 4-, 5-, and 6-body interaction energies were evaluated with BSSE corrected. For some selected sets, we calculated the energies also at RI-MP2/aug-cc-pVDZ.





The calculated *N*-body interaction energies have brought the "blocks & glues" model.



A "block" is a hydrogen bonding base-pair, meaning the hydrogen bonding energy of "1 base-pair" and there are 2 kinds of blocks. A "glue" is a stacked 2 base-pairs, meaning the stacking interaction energy of "1 stack of 2 base-pairs" and there are 10 kinds of glues.

The "blocks & glues" are composed of hydrogen-bonding and base-pair stacking interactions, and can be considered as the building units of DNA.