# Ab initio Molecular Orbital Calculation of Biomolecule

Many biomolecules have metal atoms playing important role in the biological activity. To reveal the mechanism of the biological activity at molecular level, the classical mechanical treatment is insufficient because of the flexible electronic states of metal atoms, and the quantum mechanical treatment is indispensable. The fragment molecular orbital (FMO) method treats the electronic wave-function of biomolecule explicitly, and carries out a massive molecular orbital calculation with convenient computational cost. We carried out the FMO calculation of the DNA and estrogen receptor (ER) complex, and reveal the detail interaction and the change of the ER electronic state induced by DNA binding.
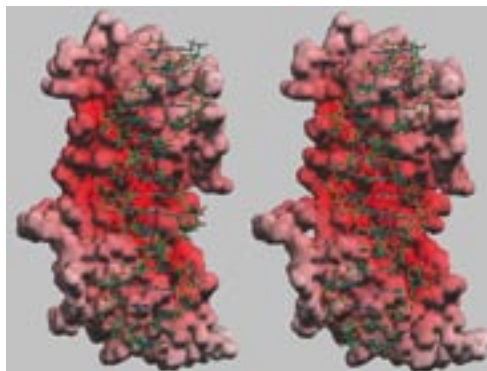

Electrostatic potentials (ESP) of the estrogen receptor: DNA binds to the largely plus ESP region (the deep red region) of the estrogen receptor. (stereovision)

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Microfluidic Conformational Changing of Macromolecule and Efficient Chemical Reaction

Conformational control of macromolecules is useful for efficient chemical and biochemical reactions. This paper reports a conformational control method for macromolecules, such as long-strand DNA, in microchannel flow, along with a simple method to stretch DNA strands by microfluidics. Stretching and orientation of DNA molecules by control of flow within a microchannel was directly observed by optical microscopy. This technique is useful to create chemical reactions with macromolecules; it offers high selectivity and efficiency that are impossible to achieve in bulk solution. We also demonstrated that our microfluidic stretching method can accomplish efficient hybridization of long-strand DNA.
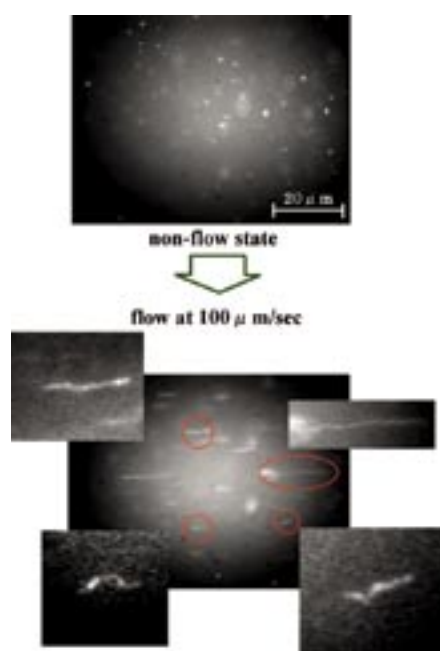
Direct observation of long-strand DNA structures in microchannel flow

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