**Innovative Simulation on Proteins** 



# F. Sato LAB.

## [Innovative Simulation on Proteins]

### **Center for Research on Innovative Simulation Software**

http://www.ciss.iis.u-tokyo.ac.jp, http://satolab.iis.u-tokyo.ac.jp

**Computational Biomolecular Science** 

#### Engineering/ Mechanical Engineering

## All-Electron Calculations on Proteins by ProteinDF

The new quantum chemical calculation software "**ProteinDF**" has been developed, where molecular orbitals of all electrons of proteins are computable.

Based on the software, a practical simulation system that precisely analyzes biomolecular reactions is now constructed for the applied research such as design of new enzymes and medicines as well as for the fundamental researches.

