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.

