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

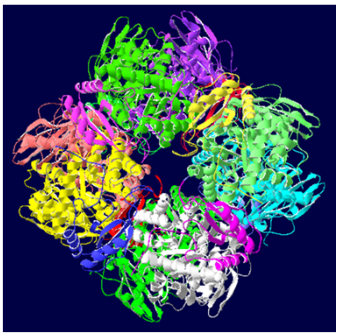
Engineering/
Mechanical Engineering

All-Electron Calculations on Proteins by ProteinDF

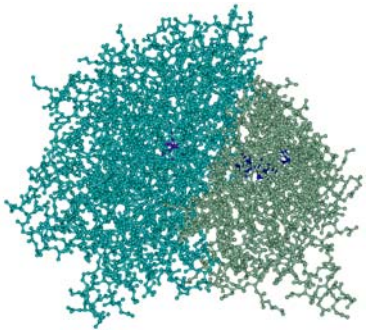
All-Electron Calculations on Proteins by ProteinDF

The new quantum chemical calculation software “ProteinDF” was developed, where molecular orbitals of all electrons of proteins are computable.

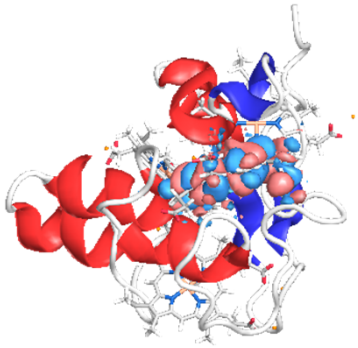
Based on the software, a practical simulation system that precisely analyzes biomolecular reactions is now constructed for the applied research such as design of new enzymes and medicines as well as for the fundamental researches.



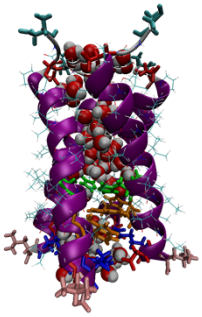
Rubisco
Highly Efficient Carbon Fixation Reaction



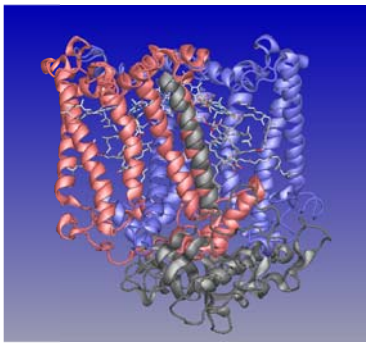
Hydrogenase
Oxygen Tolerant Hydrogen Generation



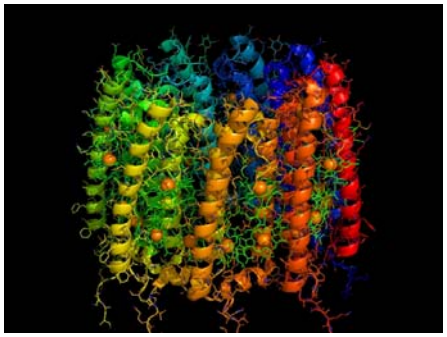
Cytochrome c_3
Redox



M2 protein
Antiviral Drugs for Influenza



PSRC
Charge Separation



Light Harvesting Complex
Light Energy Collection