

F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]

Center for Research on Innovative Simulation Software

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

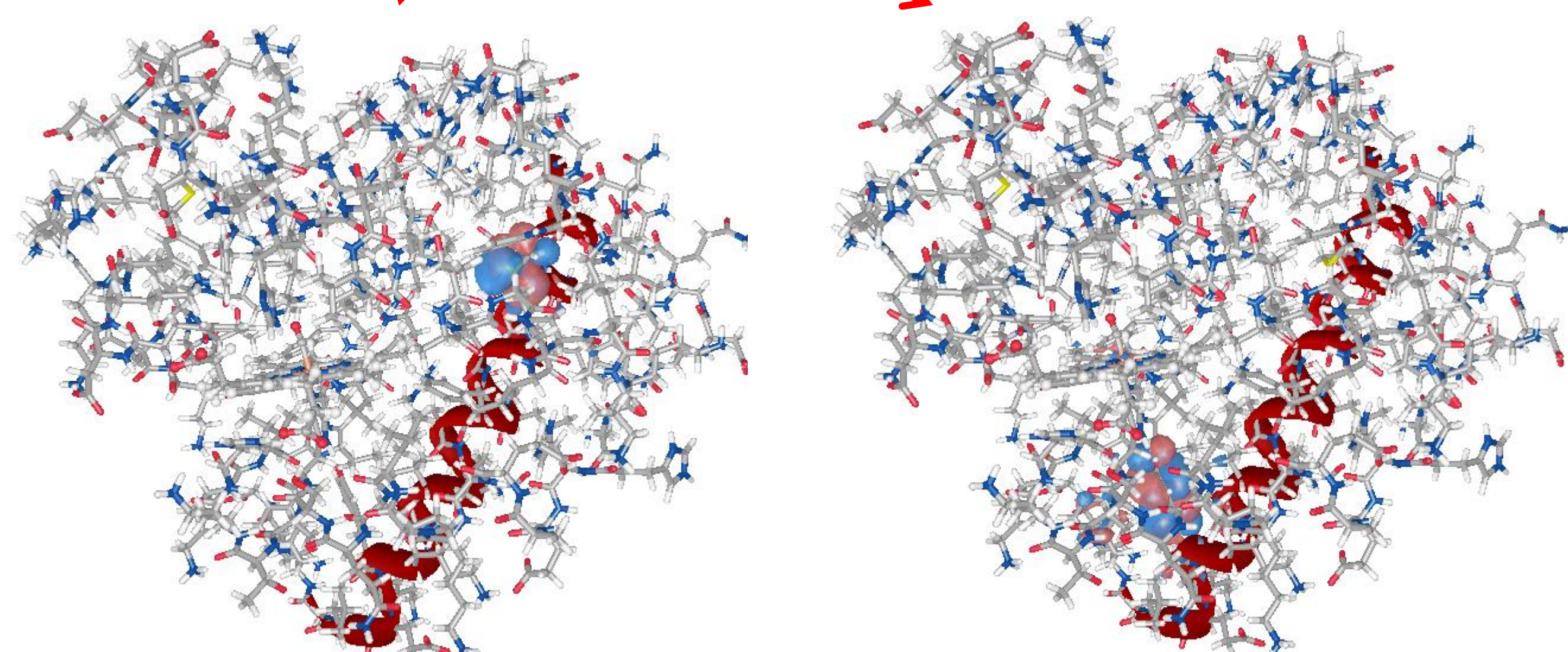
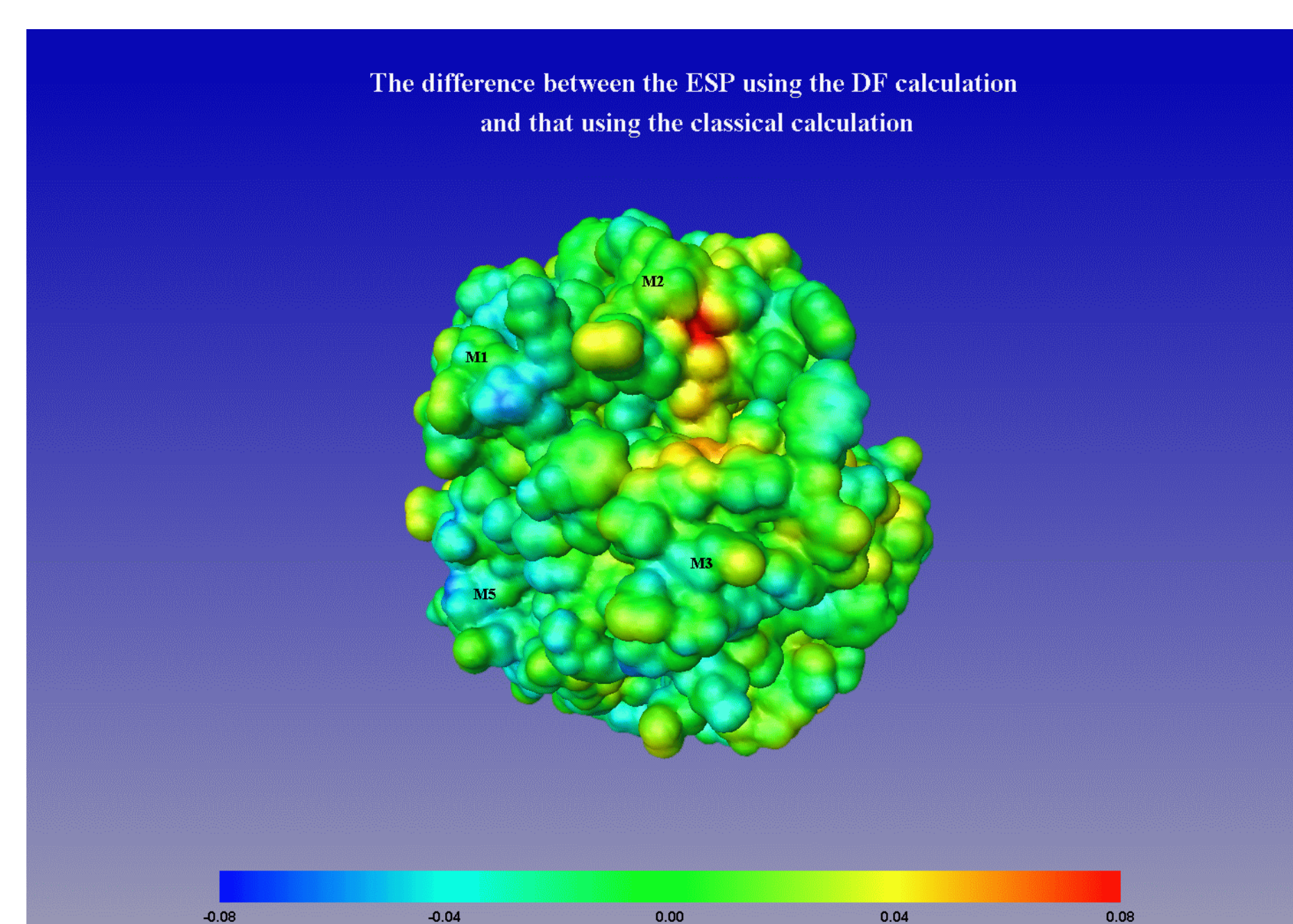
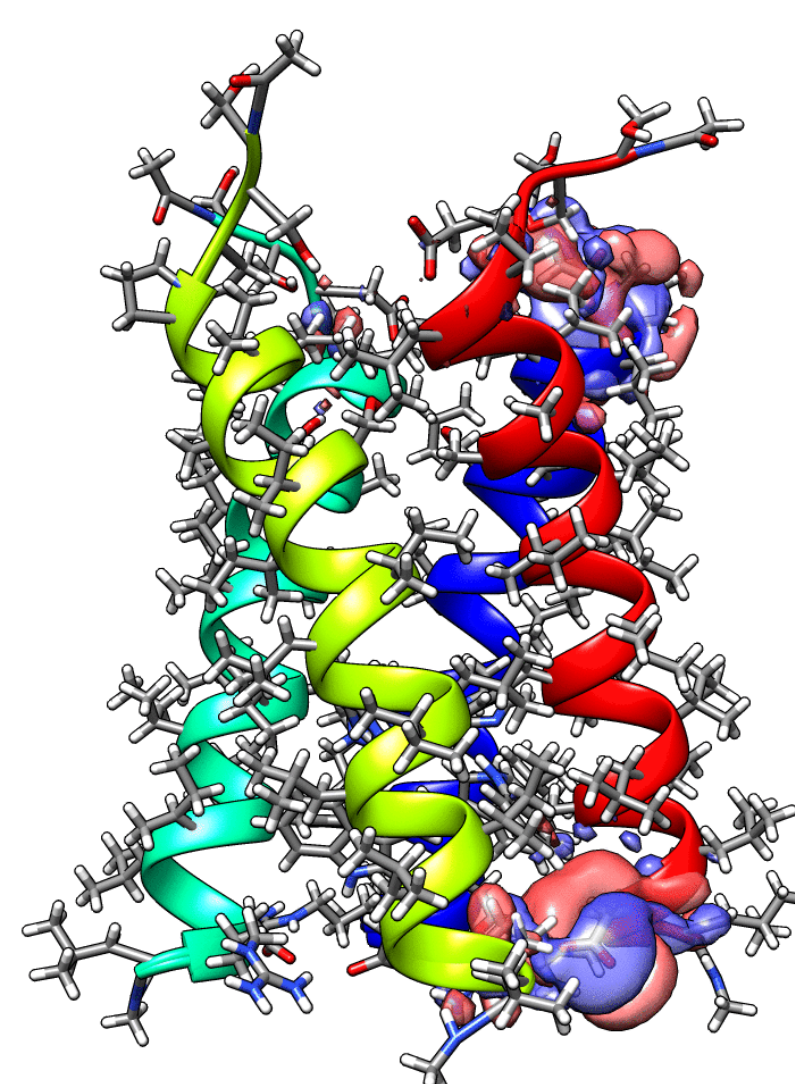
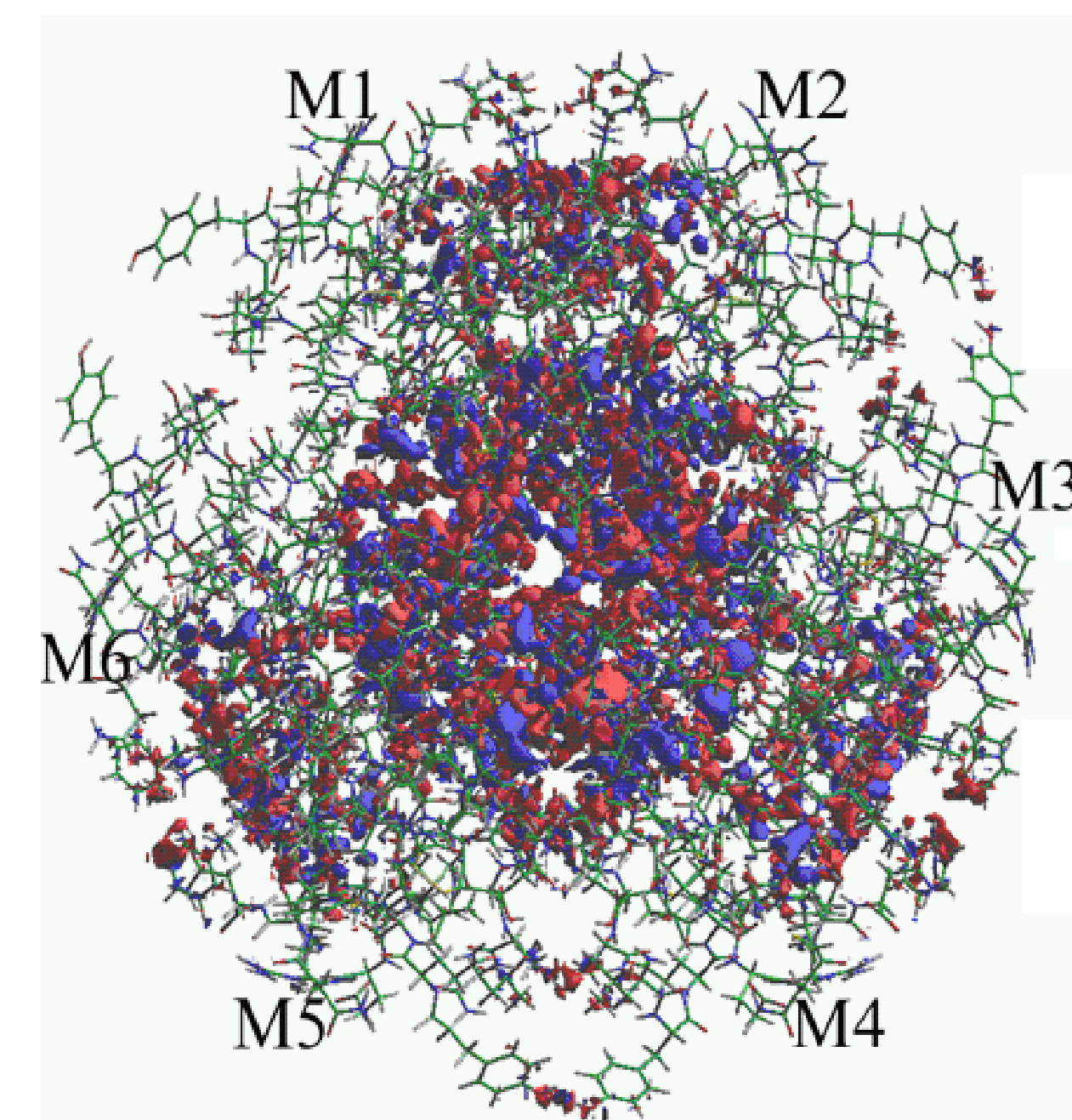
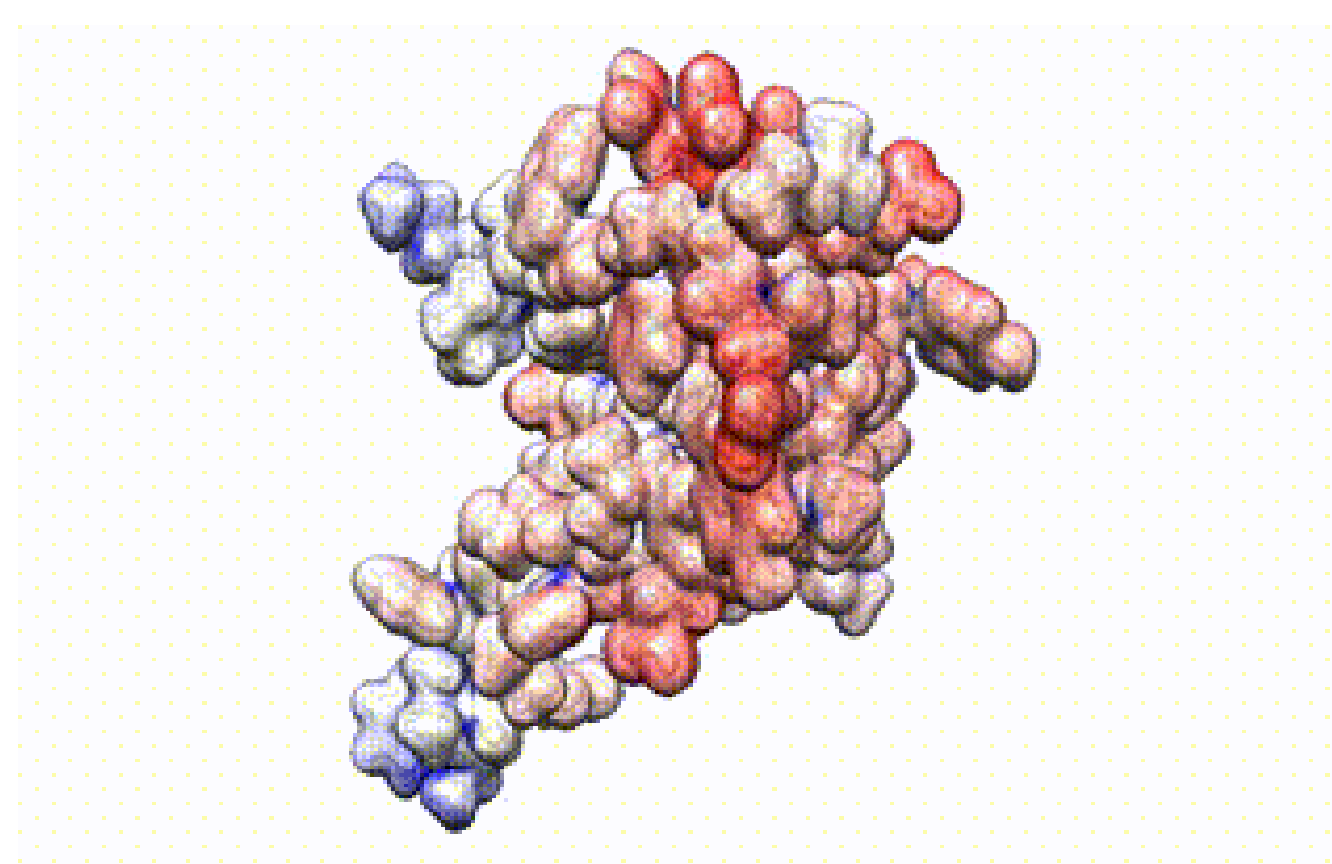
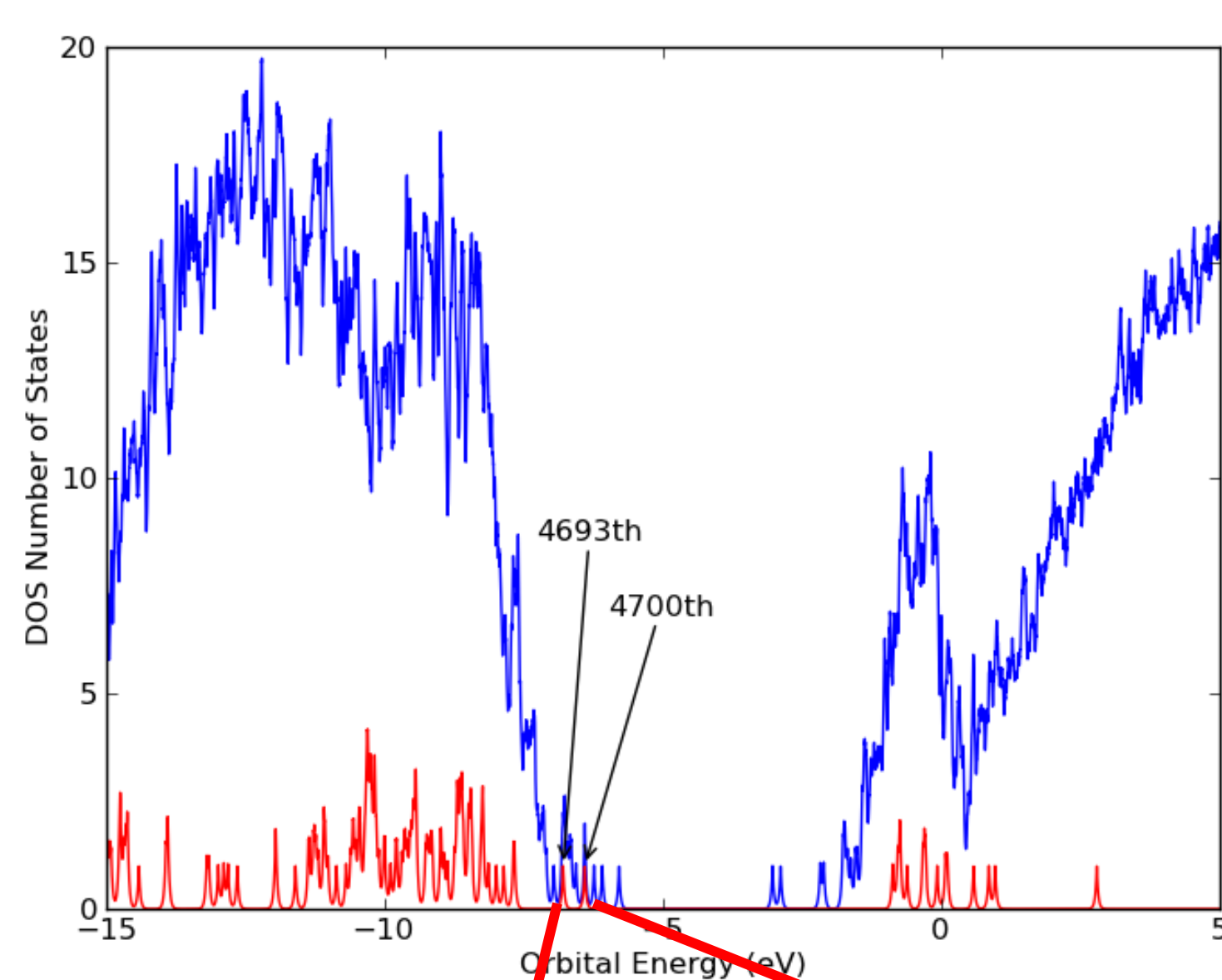
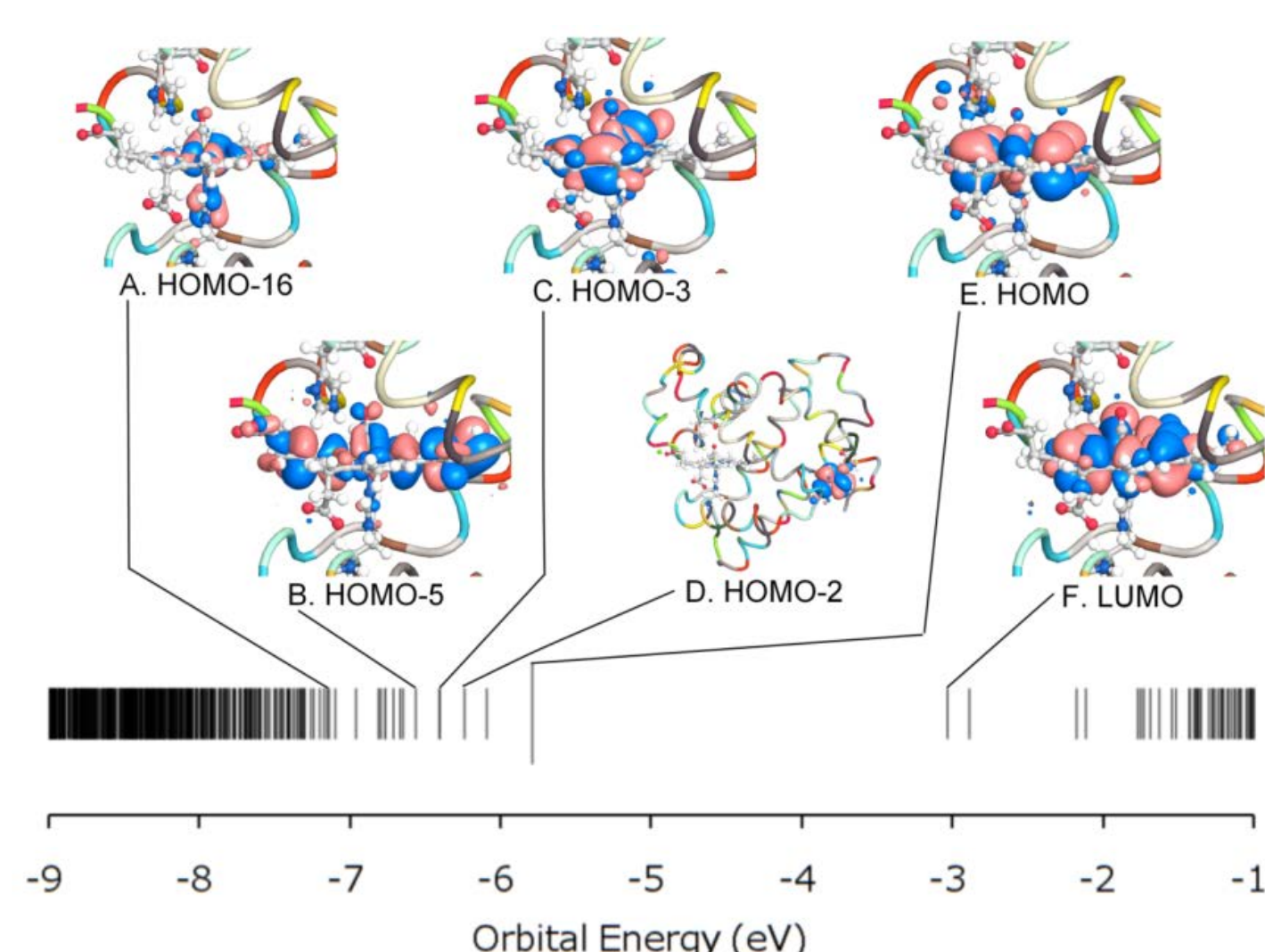
Engineering/
Mechanical
Engineering

Computational Biomolecular Science

All-Electron Calculations on Proteins by ProteinDF

The new quantum chemical calculation software “ProteinDF” has been developed, where **molecular orbitals of all electrons** of nanoscale molecules such as proteins are computable.

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



Textbooks (Japanese)