F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]

Center for Research on Innovative Simulation Software

Computational Biomolecular Science

Mechanical Engineering department

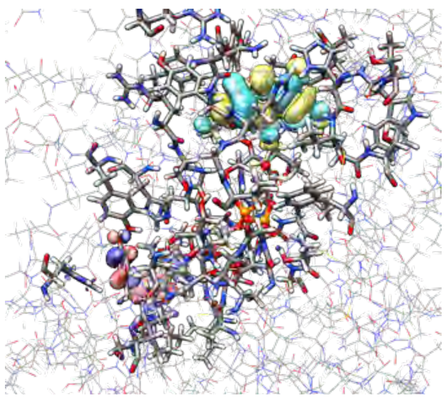
http://www.ciss.iis.u-tokyo.ac.jp, http://www.satolab.iis.u-tokyo.ac.jp

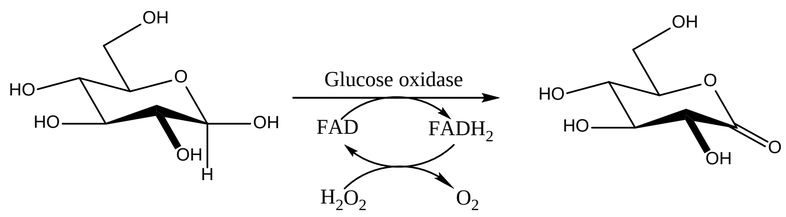
Large-Scale Canonical Molecular Orbitals Study

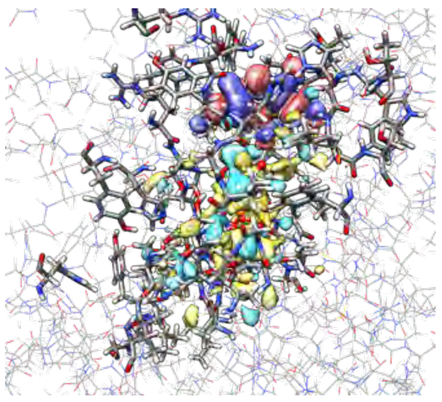
Has Great Potential in Shaping the Future.

The new quantum chemical calculation software “ProteinDF/QCLO” has been developed, where canonical molecular orbitals of all electrons of nanoscale molecules such as proteins are computable. https://proteindf.github.io/

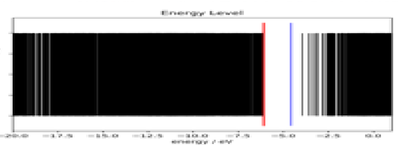
MOs

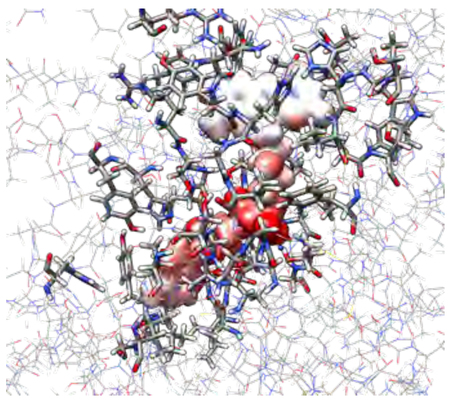






Orbital energy levels





ESP potential on the FAD surface

FAD

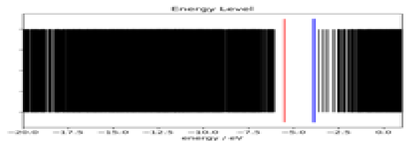
Neutral form (0)

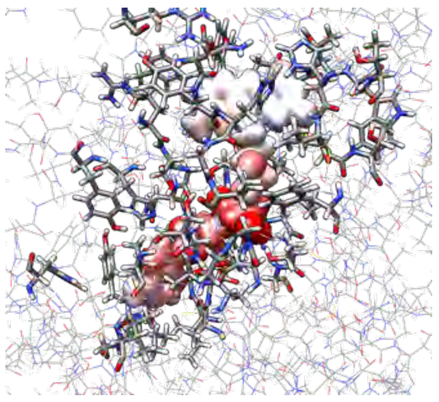
Oxidation form — FAD

Semi-quinone form

Reduction form — $FADH_2$

Negative form (1-)

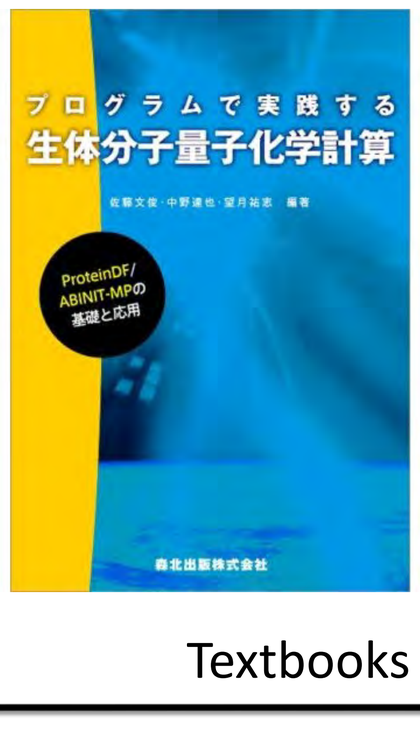




$FADH_2$

ESP potential on the $FADH_2$ surface

Electronic structure of the active site on glucose oxidase



Textbooks (in Japanese)