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

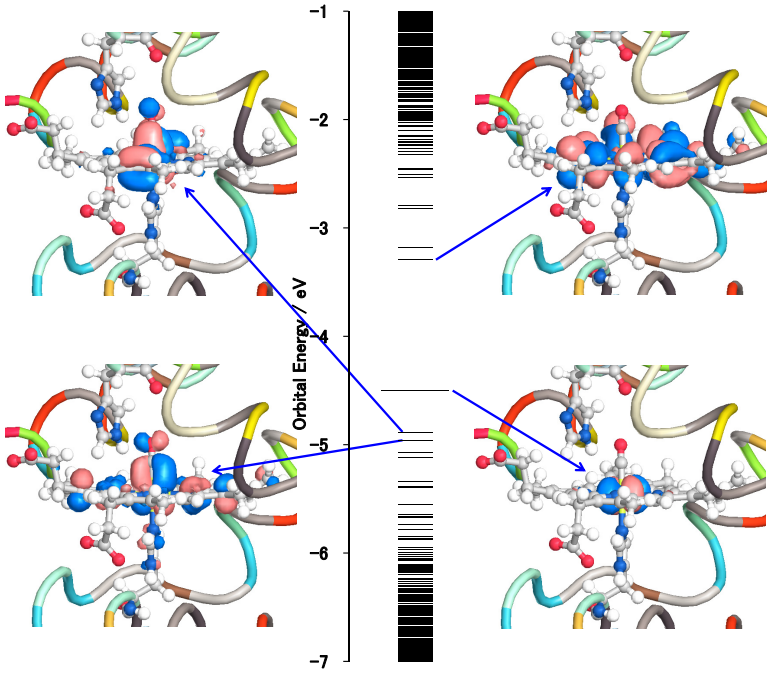
Computational Biomolecular Science

Engineering/
Mechanical Engineering

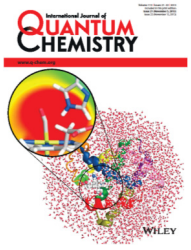
All-Electron Calculations on Proteins by ProteinDF

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.

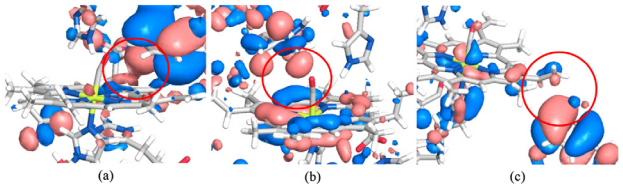


MOs of MbCO

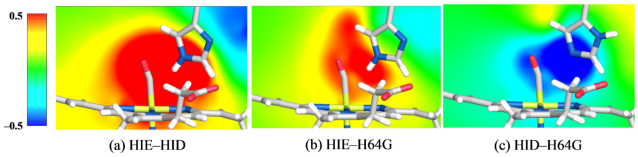


← For details

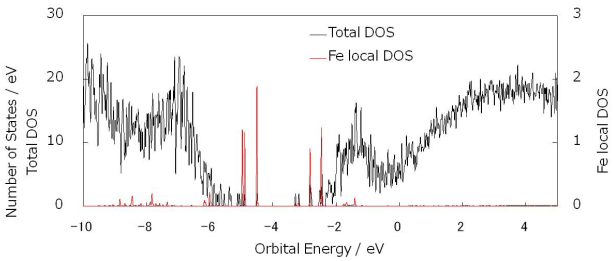
if you are interested:
T. Hirano, F. Sato, *PCCP*, 2014.
DOI: 10.1039/C3CP55514C.



The role of amino acid residues



The effects of mutation and tautomer



Analysis of DOS

Various textbooks (Japanese)